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*DEPARTMENT OF
CHEMISTRY*

HONOURS

2025

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CHEMISTRY HONOURS – 2025
Head of the Department: Prof R Klein (r.klein@ru.ac.za)
Course Coordinator: Mrs Joyce Sewry (j.sewry@ru.ac.za)

1. GENERAL CONDITIONS

1. Admission to the final examinations of the Honours course is subject to satisfactory performance in all parts of the course during the year.
2. The Chemistry Department expects all Honours students to act as Demonstrators and Tutors (as part of their bursary obligations, or for payment, as appropriate). Demonstrating and tutoring provide valuable teaching experience. Funding for tutoring & demonstrating is determined annually by the university.
3. Permission is needed to study any other courses during the year or to take up any other form of employment.
4. Honours students are expected to be on campus every day during RU terms. A Leave of Absence (LOA) must be applied for through the Chemistry Administration office in case of illness or other emergency as noted in the student disciplinary code.

• DP REQUIREMENTS

Chemistry Honours students must:

1. participate in ALL chosen lectures, and must submit ALL assessments.
2. attend ALL seminars in the Chemistry Department.
3. work on the project while not in lectures.
4. submit all submissions by the relevant dates.
5. attain a subminimum of 50% in EACH of the research project and theory respectively.

• FINANCIAL ASPECTS

Each student is responsible for financing his or her studies.

Fees for Honours:

The student fees booklet for 2025 can be found at:

https://www.ru.ac.za/media/rhodesuniversity/content/finance/documents/2025_RU_fees_booklet.pdf

The Initial Fee Payment:

Tuition only: R6 950.

Or

Tuition and Residence: R6 950.00 + R23 905.00 = R30 855.00

Other minor administrative fees may apply, such as Application Fee of R100.

International Levy and payment options, please refer to fees booklet.

HONOURS RESOURCES

All resources for the Chemistry Honours course should be available on RUConnected: You will have access to this site once you have registered.

<https://ruconnected.ru.ac.za/course/view.php?id=10533>

2. PROVISIONAL PROGRAMME FOR ORIENTATION WEEK

4 – 7 February 2025

(ALL DATES ARE PROVISIONAL AND CHANGES MAY BE MADE TO THE PROGRAMME)

Tuesday 4 February

- 09h00 Introductions: Staff and Honours students
 General outline of the Honours Course
 Introduction to the Review Essay and research projects with all staff to be led by Prof R Klein* (See also the attached handout on Writing a Scientific Report, Appendix 2.)
- 11h00 Experiences of former Honours students
- 14h00 An introduction to Reaxys Prof Klein

*POINTS FOR DISCUSSION

- What is meant by "RESEARCH"?
- What is expected in an Honours Project?
- Starting a project
- Lab notebooks
- Writing up
- Seminar with East Cape Universities
- Responsibilities of a Supervisor
- Responsibilities of the Student
- Practical problems
- Psychological problems
- Plagiarism (complete and submit form, Appendix IV)

Wednesday 5 February

Morning: Do administrative registration at Student Bureau AND academic registration with the Dean

Prepare a 2-page essay on yourself and your undergraduate studies.

Contact staff to finalise project, lecture and essay topic choices. (See email addresses later in this document)

NB You will NOT be able to choose a topic unless you have spoken to the supervisor

Afternoon Teambuilding: Details to follow

Thursday 6 February

09h00 Submit final choices of topics, projects and essays; find link on RUConnected

Submit plagiarism declaration to Chemistry administration office

09h30 - 13h00 Tutor Training (Prof Klein, Dr Tshiwawa)

16h00 STAFF ONLY Meeting (finalizing of Honours programme and project and essay allocations).

Friday 7 February

09h00 Library workshop (venue: Xstrata lab, RU Library). Meet Ms Menze in the library Foyer, level 1

Please see Link below for the Library Website Tutorial Videos: [Virtual Tour](#)

17h00 Hand in your essay on yourself by email to chemistry@ru.ac.za

Monday 10 February

08h00 **Lectures begin for all Honours students**

A DRAFT Timetable will be provided as early as possible. This is likely to be changed from time to time. See RUConnected for the Timetable. Also see the Honours noticeboard in the Chemistry tearoom.

Honours students also to start on their essays.

Tuesday 11 February

14h00 Demonstrator training for all postgraduates (Prof Klein, Dr Tshiwawa)

3. PROGRAMME FOR 2025

Important activities

Dates To be Confirmed (TBC) for activities below

Summary of important dates (by Term):

First Term:

- Oral presentation of project plan: **early in first term**
(Each student will have been given key papers related to his/her project. Please read these papers carefully and prepare a short talk (10 min maximum) on your **plan for the project**.
(see the attached Appendix on “Giving an Oral Presentation”)
- Safety test: **Friday of first week of lectures**
- Hand in 1st draft of essay: **end of 1st Term (13h00 on 28 March)**

Second term:

- 1st draft of essay back from supervisor: **beginning of 2nd term (7 April)**
- Oral presentation of essays: **provisionally 2 weeks before SWOT week (provisionally 5 May)**
- Mid-year research group project seminars: Last week of 2nd term, arranged within research groups)
- Hand in final version of essay: **Last day of lectures in 2nd Term (17h00 on 16 May)**
- Tutor refresher (TBC)
- Mid-year exam: **June; dates to be determined by Registrar’s division**

Third term:

- Collect June scripts and discuss the exam results with lecturer concerned

Fourth term:

- Hand 1st draft of project: **1st day of 4th Term, 25 August 2025**
 - Project seminar: **provisionally 8 September 2025**
 - Hand in Final version of project report: **17h00 on 15 September 2025**
 - Final Honours examinations: **November; dates to be determined by Registrar’s division**

4. ACADEMIC STAFF INVOLVED IN CHEMISTRY HONOURS



Prof Rosa Klein (RK),
Head of Department



Prof Philani Mashazi
(PNM)



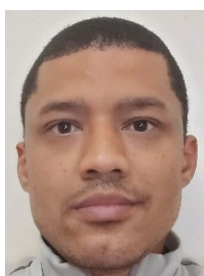
Dist Prof T Nyokong
(TN)



Prof Kevin Lobb
(KAL)



Dr Vincent Smith (VS)



Dr Theo Geswindt
(TG)



Mrs Joyce Sewry (JS)



Emeritus Prof Gary
Watkins (GW)



Dr Tendamudzimu
Tshiwawa (TT)



Dr Mpondi Molefe
(NFM)



Dr Kabelo Ramollo (KR)



Prof John Mack (JM)



Dr Jonathan Britton (JB)

5. DETAILS OF THE HONOURS COURSE

Purpose and characteristics

The Bachelor of Science (Honours) Degree is a postgraduate specialisation qualification, characterised by the fact that it prepares students for research based postgraduate study. This qualification typically follows a Bachelor's Degree, and serves to consolidate and deepen the student's expertise in a particular discipline, and to develop research capacity in the methodology and techniques of that discipline. This qualification demands a high level of theoretical engagement and intellectual independence. In some cases, a Bachelor of Science (Honours) Degree carries recognition by an appropriate professional or statutory body. Bachelor of Science (Honours) Degree programmes must include conducting and reporting research under supervision, worth at least 30 credits, in a manner that is appropriate to the discipline or field of study.

Honours is an NQF Exit Level 8 qualification, with a minimum 120 credits, of which 120 credits (~1200 notional hours) have to be at NQF level 8, and includes approximately 30 credits of supervised research.

Approximate credit breakdown of the course:

	Credits(hours)	Comments
Research Project	35(350)	~20 h per week for 3 terms
Review Essay	5(50)	~5 h/week for 1½ terms
Theory	80(800)	For each hour of lectures, at least 4 h self-study

COURSE STRUCTURE

(A) Theory: Lecture topics (15 topics to be chosen):

Topics are selected by the student from the list attached, subject to the approval of the Chemistry staff, to ensure a well-rounded curriculum. Students should consult the project topics for recommendations on lectures needed.

The topics vary from year-to-year depending on staff availability and their interests, and on the number of students selecting the topic.

(B) An introductory research project:

This is done during the first three terms under the supervision of a member of staff in a field selected by the student from projects offered by staff members. Students are required to give short talks on their projects at a Departmental seminar in September or October. One or two of these talks will be selected for an oral presentation at a joint SACI (South African Chemical Institute) seminar with the three other Higher Education Institutions in the Eastern Cape, Nelson Mandela University (NMU), Walter Sisulu University (WSU) and University of Fort Hare (UFH).

(C) A review essay:

An essay of approx. 3000 words (10-15 x A4 pages), on a topic not associated with the project, is written in the first and second terms under the supervision of a staff member (other than the one concerned with the project). The first draft of the essay must be kept, and the final mark will take the first draft into consideration.

Joint Honours: Chemistry/Another Science subject

It is possible, at the discretion of the departments concerned, for students to do Joint Honours in Chemistry and another subject. For Joint Honours, each of the component subjects must make up at least 40% of the total course. The composition must be specified in writing and agreed to by the Heads of both Departments. Joint Honours will only be available as an option to students who achieve a 1st class pass for their Chemistry 3 course.

Modules from other courses?

With permission from the Heads of Departments (HoDs) of both Departments, it is possible to swap up to 3 elective modules in Chemistry with modules from the Honours Course of another Department, provided the Credit value is approximately the same.

6. COURSE ASSESSMENT

(Total marks: 1000)

ONE 3-hour paper is written in June. This examination serves as a guide to students and staff as to whether satisfactory progress is being made. Where progress is not satisfactory, candidates may be advised to spread the Honours degree over two years, or to withdraw.

Students who obtain less than 50% on any question(s) answered, are required to review the question(s) with the relevant lecturer early in the third term. However, the marks obtained during the June Examination, will count.

The final examinations are written in November. There are **three 3-hour papers**. Each paper covers the material dealt with in FIVE of your topics; (see list under LECTURE TOPICS). You are required to answer a maximum of FOUR of the questions in each paper. As in all examinations, equal time, in this case 45 minutes, should be allocated to each answer. An option of up to two modules that are evaluated by continuous assessment may be taken per paper. A minimum of NINE topics need to be answered in the examinations.

A subminimum of 50% in each of the research project and theory respectively must be attained to pass Chemistry Honours.

Component	Sub-component	Marks	% of total mark
June theory exam		60	6 %
Project:		Total:250	25 %
	Presentation	30	
	Written report	220	
Essay:		Total: 150	15 %
	Presentation	20	
	Essay hand-in	130	
Theory:	12 modules: 4 each in 3 papers	12 x 45 = 540	54 %
TOTAL		1000	100 %

7. LECTURE TOPICS (A)

FIFTEEN topics must be chosen from the list below (a detailed explanation of the topics is given on the pages which follow). It is impossible to allow a perfectly free choice of topics. The topics are thus listed in **FOUR** groups (see below). A **maximum of FOUR topics from each paper** must be chosen. No more than **ONE** additional topic in each section may be selected initially and the final **FIFTEEN** must be confirmed *in writing* before the end of May. A maximum of FOUR topics will be answered in each exam paper. A minimum of **NINE** topics need to be answered in the examinations. Complete the form at <https://docs.google.com/forms/d/1TvbQM3S5s824oRu4bYXWJK6MJnssaOKQ3gm8G19PHWQ>
Details of topics follow below the table.

<u>Paper 1</u> <u>Max 4</u>	VS1	Solid State Properties of Materials
	PNM1	Intelligent nanomaterials and their applications
	GW2	Vibrational spectroscopy
	NFM2	Chemistry of Liquid Crystals
	RK3	Advanced retrosynthesis and Green Chemistry
	KR1	Catalysis
<u>Paper 2</u> <u>Max 4</u>	TT1	Applications of Statistical Thermodynamics
	JM2	Porphyrinoid chemistry
	PNM2	Design and development of biosensors
	NFM3	Inorganic reaction mechanisms
	RK1	Asymmetric Synthesis
	TG2	Separation science – From fundamentals to modern trends
<u>Paper 3</u> <u>Max 4</u>	JS1	Introduction to Chemometrics
	EA1	Solid State NMR
	KAL1	NMR spectroscopy
	JM3	Optical spectroscopy
	GW1	Symmetry and group theory
	VS2	Supramolecular Chemistry
<u>Continuous Assessment</u> <u>Max 4</u>	VL1*	Industrial Perspective of Analytical Chemistry
	KAL3	Molecular Modelling: Interactions and Dynamics
	JS2*	Service-Learning in Chemistry
	JM1	Molecular Modelling: molecular symmetry and TD-DFT
	TT2	Ethnochemistry
	TG1	Advanced kinetic analyses

In addition: RK2 Introduction to Research Methods. (NOTE this is a REQUIRED topic for all students)

The aims of this course are to explore techniques which are not covered in undergraduate practical courses as well as encourage students to develop skills in synthetic experiment design, and in critical analysis of experimental outcomes. The course will combine theoretical principles with practical experimentation in the context of equipment and opportunities available within the department.

- Topics in the last block are examined by various “in course” (continuous) assessments.
- *Topics indicated in **bold** are required modules.

- A minimum of two examinable topics are required per paper, and a minimum of two (with a maximum of three) continuous assessed courses are required in total.
- A student who selects continuous assessment modules and does NOT submit assignments etc. or drops out mid-way from the course will get the mark they obtained UP TO THAT POINT, which could be zero. This is equivalent to selecting a module to write in the exam and not writing anything.

One paper in another major subject

It is possible for up to five Chemistry topics to be replaced by an equivalent amount of material in another subject, by arrangement with the Heads of Departments concerned. In this case the degree remains Chemistry Honours. Alternatively, some Chemistry topics may be chosen in an Honours degree in another subject. All such combinations must be specified in writing and approved by the Heads of both Departments concerned. A full joint Honours will only be available as an option to students who achieve a first class pass for 3rd year chemistry.

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DETAILS OF LECTURE TOPICS

PAPER 1

DR V J SMITH

VS1 The Solid State Properties of Materials

Solid state properties are key to understanding the physical behaviour of materials and to ensure optimal physical form. Moreover, the selection of optimal form is a critical aspect in the development of new materials (pharmaceutical or other). In this course we will cover the various aspects of solid state characterisation of materials.

PROF P MASHAZI

PNM1 Intelligent nanomaterials and their applications

There is a current global trend growing in the application of nanomaterials in various industries. The interest has been sparked by the intrinsic properties that nano-sized and nano-structured materials exhibit. Various interests in the application of nanomaterials look into solutions these materials may provide into current day challenges. These materials can be intelligently designed to target specific applications.

The examples are that these materials are investigated for their potential as vehicles for targeted drug delivery, enhancement of electrical signals in sensor applications, visualisation in point-of-care diagnostic tests, heterogeneous catalysts for industrial applications (such as catalytic converters, carbon monoxide oxidation, etc.), miniaturized systems for space applications, the list is endless. The module will look at different types of nanomaterials, their design for targeted applications, properties and their effect when tested for these specialized applications.

DR NF MOLEFE

NFM2 Chemistry of liquid crystals

The study of liquid crystals began in 1888 when an Austrian botanist named Friedrich Reinitzer observed that a material known as cholesteryl benzoate had two distinct melting points. In his experiments, Reinitzer increased the temperature of a solid sample and watched the crystal change into a hazy liquid. As he increased the temperature further, the material changed again into a clear, transparent liquid. Because of this early work, Reinitzer is often credited with discovering a new phase of matter - the liquid crystal phase.

A liquid crystal is a thermodynamic stable phase characterized by anisotropy of properties without the existence of a three-dimensional crystal lattice, generally lying in the temperature range between the solid and isotropic liquid phase, hence the term mesophase. Liquid crystal materials are unique in their properties and uses. As research into this field continues and as new applications are developed, liquid crystals will play an important role in modern technology.

Emeritus PROF G M WATKINS

GW2 Vibrational spectroscopy

A non-mathematical introduction to infrared and Raman spectroscopy and instrumentation. The application of some techniques employed in the assignment problem. (Some knowledge of Group Theory, covered in GW1, is necessary for this topic.)

PROF R KLEIN

RK3 Advanced retrosynthesis and green chemistry

In September 2015 the United Nations adopted the Sustainable Development Goals. As chemists we can make a substantial contribution to the changes which are necessary to address climate change, poverty alleviation and sustainability in general. This course will look at the application of retrosynthesis as a tool to highlight opportunities to use bio-derived compounds as renewable resources in synthesis, and the application of a set of green chemistry metrics to assess our synthetic processes.

DR K RAMOLLO

KR1 Catalysis

Catalysis is one of the most economically important areas of chemical practice and research. This course will include an overview of homogenous and heterogeneous catalysts used in organic chemistry. An emphasis will be placed on processes which are used industrially, and those which yield asymmetric products. Selected mechanisms will also be considered

PAPER 2

Dr T Tshiwawa

TT1 Applications of Statistical Thermodynamics

This section focuses on the application of statistical thermodynamics concepts to the calculation of chemically significant quantities. First, we establish the relations between thermodynamic functions and partition functions. Next, we show that the molecular partition function can be factorized into contributions from each mode of motion and establish the formulae for the partition functions for translational, rotational, and vibrational modes of motion and the contribution of electronic excitation. These contributions can be calculated from spectroscopic data. Finally, we turn to specific applications, which include the mean energies of modes of motion, the heat capacities of substances, and residual entropies. In the final section, we see how to calculate the equilibrium constant of a reaction and through that calculation understand some of the molecular features that determine the magnitudes of equilibrium constants and their variation with temperature

Prof J MACK

JM2 Porphyrinoid chemistry

The synthesis, characterization, properties and applications of BODIPY, porphyrin and phthalocyanine dyes will be explored with a strong emphasis placed on research topics that are directly relevant to the Institute for Nanotechnology Innovation. The module is designed to provide students contemplating a career in chemistry with examples of how the theory learned during undergraduate chemistry courses can be applied in a research and development environment to solve practical problems and create new industrial and biomedical products.

PROF P MASHAZI

PNM2 Design and development of biosensors

Early detection of pollutants and pathogens in environmental, biological and industrial samples is a subject of international interest. The surveillance and control of the spread of these harmful substances that may be harmful to humans, microorganisms and the environment will be discussed. This will then highlight the need for systems that may be effective and accurate in detecting and/or monitoring the levels of these undesirable substances from the various samples. In the environment and biological systems these hazardous substances possess a big threat to human and animal health. Therefore, to improve the quality of life for humans, detection and monitoring of these hazardous substances at an early on-set of infection or contamination is important. The detection and monitoring systems are important for effective and timeous treatment and as early warning systems. The material covered in this module will be the systems currently used and those that are under development by various institutions for detection and monitoring of the substances harmful to the environment and biological systems. The design and development issues arising from the semi-commercial systems will also be discussed whilst highlighting the successes of other systems. Different techniques will be discussed and their impact in the cutting-edge of the bio/sensor technologies to impact the future in industrial applications

DR NF MOLEFE

NFM3 Inorganic reaction mechanisms

Transition metal ions and complexes play a fundamental role in at least three areas of research: (i) bioinorganic chemistry and molecular biology, in investigating the functions of metal complex metalloproteins, (ii) industrial chemistry, in exploiting metal complexes as homogeneous catalysts for the optimization of very important commercial processes, such as polymerization, hydroformylation, hydrogenation, oxidation of olefins, etc., (iii) environmental and medicinal chemistry. Understanding the mechanism of the reactions at transition metal sites is then crucial in designing new inorganic materials, developing industrial homogeneous catalysts, and gaining insight into the role of metalloenzymes in biological processes and metals in medicine.

A mechanism is then a predictive theoretical construction that account for all the kinetic, spectroscopic and theoretical information currently available on a reaction. (INORGANIC AND BIO-INORGANIC CHEMISTRY – Vol. II - Inorganic Reaction Mechanisms - Raffaello Romeo)

PROF R KLEIN

RK1 Asymmetric synthesis

An introduction to the principles of asymmetric synthesis and a survey of current methodologies for the synthesis and analysis of chiral compounds.

DR T GESWINDT

TG2 Separation science – From fundamentals to modern trends

A good knowledge of separation techniques becomes ever more necessary, as separating (complex) mixtures into their components is applied across all disciplines of chemistry and related sciences.

In this course, the fundamental aspects of chromatography will be discussed – with the aim of moving to more modern trends in separation techniques (two-dimensional techniques, hyphenation *etc.*)

PAPER 3

MRS JD SEWRY

JS1 Introduction to chemometrics

“Chemometrics is the chemical discipline that uses mathematical and statistical methods, (i) to design or select optimal measurement procedures and experiments, and (ii) to provide maximum chemical information by analysing chemical data.” Matthias Otto.

The course does an overview of basic statistics and then looks at experimental design and finding optimal conditions

PROF E ANTUNES (VISITING FROM UWC)

EA1 Solid State NMR

Solid state Nuclear Magnetic Resonance (NMR) is a technique for characterizing the structure and dynamics of matter at atomic scale e.g., powders, single crystals, and amorphous samples. Unlike in solution state NMR, anisotropic spin interactions are present in the solid state causing larger linewidths. Techniques that can be used to deal with these interactions will be discussed, as well as the quantitative information that can be derived on molecular structure, conformation, and dynamics of materials. This course will also highlight the usefulness of NMR spectroscopy for the characterization of organic molecules, proteins, and advanced materials.

PROF K LOBB

KAL1 NMR spectroscopy

The practical application of 1D and 2D Fourier transform NMR techniques commonly used to determine the structures of organic molecules. Where applicable, theoretical aspects of modern NMR techniques will be described using a largely non-mathematical approach.

PROF J MACK

JM3 Optical spectroscopy of aromatic π -systems and transition metal complexes

The analysis of optical spectral data (including circular dichroism, magnetic circular dichroism and emission spectroscopy in addition to electronic absorption spectroscopy) of aromatic π -systems and transition metal complexes is explored. A strong emphasis will be placed on the information that can be derived on the structure and properties of heteroaromatic molecules and transition metal complexes in a manner that is potentially directly relevant to research project work.

PROF G M WATKINS

GW1 Symmetry and Group Theory

(NOTE: this is a required topic for all students.)

Symmetry and point groups. The methods of group theory are applied to simple molecules with reference to hybrid orbitals and in the interpretation of vibrational and electronic spectra. (This is a largely non-mathematical introduction to the subject)

DR V SMITH

VS2 Supramolecular Chemistry

Defined as the “Chemistry beyond the molecule”, supramolecular chemistry explains how molecules and ions join together in fascinating structures using only intermolecular forces. These entities range from tiny to enormous and have many applications from explaining why lizards can stick to walls, to data-storage, to robotic nano-devices that can deliver medicines like futuristic machines.

In this module we will explore some of the recent developments in supramolecular chemistry with a focus on techniques that you can use to identify and construct your own supramolecules.

The module is driven by YOUR interests using experiments, literature, and discussions.

CONTINUOUS ASSESSMENT

These topics will not have questions in the formal examinations, but will be assessed throughout the year.

VISITING LECTURER Dr Heidi Duveskog, Director of Contextualize (Pty) Ltd

(NOTE: this is a required topic for all students.)

VL1: Industrial Perspective of Analytical Chemistry

The course highlights the multi-faceted role of Analytical Chemistry in Industry and the Environment, giving an overview of how Analytical Chemistry is applied across a value chain of processes. The module introduces the various technologies and stakeholders encountered in the workplace, including working hands-on with tools like video conferencing. This addresses an understanding of the technical component of their area of expertise (concepts such as 'detection limits' and statistical tolerances associated with results), as well as the business component and the ability to use results to influence decision making. Participants will have the opportunity to work through case studies to see how these components come together to establish core competencies within industry. Assessment will be by continuous assessment, with peer review and feedback (from team projects and presentations). **This course is compulsory.**

PROF K LOBB

KAL3 Molecular Modelling: Interactions

This is a practical course but with a focus on medicinal chemistry. Construction of models is addressed followed by a general background to molecular mechanics and *ab initio* methods, with focus on molecular mechanics and conformational searching. QM/MM methods are also included. The algorithms used in docking small molecules to active sites of enzymes are presented, followed by practical aspects of working with the docking software and the analysis of results. (Continuous assessment will involve the completion of a small project in lieu of an exam question.)

MRS JD SEWRY

JS2 Service-Learning in Chemistry

(NOTE: this is a required topic for all students.)

This course will entail one lecture on an Introduction to Service Learning. Thereafter, the students will have to work in groups and do the Service-Learning module, working with the Mobile Science Lab (MSL). The idea is that the chemistry students will work in groups of 2 or 3, with staff of the MSL. Together, they will identify relevant practicals for schools. The students will make a video of the practical being performed. The video will then be available for distribution to the Makhanda schools, and for use by the MSL

PROF J MACK

JM1 Molecular Modelling: molecular symmetry and TD-DFT calculations

Density functional theory (DFT) can be used to derive optimized geometries for newly synthesized molecules, such as phthalocyanines, porphyrins and BODIPY dyes, which in turn can be used to carry out time-dependent density functional theory calculations (TD-DFT) so that trends in the optical and redox properties can be identified. The course will provide hands on experience with calculations of this type, which will enable students to use a rational approach in identifying target compounds for synthesis work with properties that are likely to be appropriate for specific applications.

TT2 Ethnochemistry – Continuous Assessment

Indigenous knowledge is becoming increasingly important in chemistry, especially in relation to the possibility of isolating compounds valuable for drug development from plants utilized in traditional medicine. This has opened the doors to the exploration of other aspects of chemistry-related practices (practices based on the knowledge of properties of substances and materials) in indigenous societies. In this module we will focus on the traditional chemistry related practices among the indigenous societies, providing an overview from various application areas (household activities, cosmetics, paints and dyes, decorations, medicine etc.). At the end of the module, you will write a report that highlights the chemical knowledge embedded in these practices, also in view of a desirable incorporation of information about them into chemical education, to stimulate learners' positive attitude towards chemistry by linking it to indigenous chemical heritage.

TG1 Advanced Kinetic Analyses

In general, chemical kinetics stems from the fascinating scope of the macroscopic physical properties that chemical systems exhibit in the non-equilibrium state. These range in complexity from ligand exchange under well controlled experimental conditions, oscillating chemical reactions, pattern or structure formation and bifurcation. It is an exciting time in the field of chemical kinetics considering that, in principle, with modern computers and a fair knowledge of programming numerical algorithms, even the most complex system of differential equations can be solved. The role that chemical kinetics fulfils in nature is a testament to the importance of a detailed understanding of kinetics. This module explores the various intricacies of more complex (redox) reactions, and how to solve these systems using a combination of geometrical and numerical analyses

ON THE LAST PAGE OF THIS BOOKLET IS SPACE FOR YOU TO PLAN YOUR CHOICES.

PLEASE ENTER YOUR FINAL CHOICES at

<https://docs.google.com/forms/d/1TvbQM3S5s824oRu4bYXWJK6MJnssaOKQ3gm8G19PHWQ/>

8. RESEARCH PROJECT (B)

Introduction:

The project is intended to be an introduction to the methods of research and will thus cover as many of the following aspects as possible:

1. searching literature
2. planning experiments
3. setting up and calibrating apparatus
4. preparing, purifying and characterizing samples
5. using as many different techniques as possible to study the problem on hand
6. analysing the results of experiments
7. collating the results of different experiments
8. discussing the results in terms of theory and previous work
9. writing a report on the project as a whole
10. presenting a seminar on your research

A list of the projects being offered is supplied below. You should discuss all projects of interest with the members of staff concerned before making your final choice.

The final Research Report should be concise and care should be taken with both grammar and spelling (use the spell and grammar checker in MS Word AND use Grammarly). The report should put through Turnitin before submitting an electronic copy to your supervisor. The Turnitin report must also be submitted. A full list of references should be included. Help given by other persons in addition to the supervisor should be acknowledged. Marks for the project make up 25% of the final Honours mark. It is expected, however, that students should spend **all** their working week, outside of time spent on lectures, tutorials and demonstrating (*i.e.*, approximately 25-30 hours per week for three terms) on their project. This should be done during normal working hours, when staff are available for consultation, and for safety reasons. Other work such as reading for lecture topics, essays, prac and tutorial marking etc., should be done in the evenings. The presentation will be assessed by staff and will count for 30 of the 250 marks. A subminimum of 50% for the project is required, to pass Chemistry Honours.

The rubric for the final draft is shown in Appendix III

SEMINAR ON INTRODUCTION TO YOUR RESEARCH PROJECTS (No Assessment)

RESEARCH PROJECT DATES:

Practical Work	Start:	First week of lectures
	End:	End of 3rd term (AT THE LATEST)
Presentation of project plan		TBC
Hand in first draft		1 st day of 4 th Term
Hand in final version		15 September
Mid-year research group seminar		Last week of 2nd term
End of research project group seminar		Beginning of September
Presentation to Department		8 September

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• **RESEARCH PROJECT (SHORT TITLES) 2025**

PLEASE NOTE: Please indicate your first choice and second choice. These MUST be from different supervisors.

(<https://docs.google.com/forms/d/1TvbQM3S5s824oRu4bYXWJK6MJnsaOKQ3gm8G19PHWQ/>)

DR J BRITTON

- JBp1 Modification of supercapacitor electrodes using carbon nanomaterials and phthalocyanines/porphyrins.
 JBp2 Synthesis of ZnO and TiO₂ nanorod arrays for use in dye-sensitized solar cells in conjunction with phthalocyanines

DR T GESWINDT

- TGp1 The chemical origin of steam nano-bubbles
 TGp2 Functionalization of polymeric supports with aliphatic (poly)amines in the use of PGM separation

PROF R KLEIN

- RKp1 Exploring Multicomponent reactions – an application of green chemistry principles
 RKp2 Catalysis
 RKp3 Green polymer chemistry

DR K Ramollo

- KRp1 Reduction catalysts bearing Schiff base ligands
 KRp2 Synthesis and characterization of Fischer carbene complexes
 KRp3 Carbene complexes for homogeneous catalysis

PROF J MACK

- JMp1 Nanoparticle conjugates of BODIPY dyes for biomedical applications
 JMp2 Water-soluble porphyrin analogues for biomedical applications
 JMp3 AzaBODIPYs for optical limiting of laser light
 JMp4 BODIPY-embedded nanofibers for wastewater treatment

PROF P MASHAZI

- PNMp1 pH-sensitive nanosize liposomes
 PNMp2 Enzymatic properties of nanomaterials
 PNMp3 Octa-carboxylic acid MPcs

PROFESSOR T NYOKONG

- TNp1 Water purification using green technology
 TNp2 Development of Antibacterial agents
 TNp3 Protection of the eye and optical devices from strong laser light

MRS J SEWRY

- JSp1 Service-Learning with Mobile Science Lab
 JSp2 Tutoring at the Khanya Maths and Science Club

DR V SMITH

- VSp1 The reuse and repurposing of medicines through cocrystallization

PROF KA LOBB

- KALp1 Accurate prediction of ligand poses within protein active sites
 KALp2 Overview of the Aza-Cope rearrangement

Dr NF MOLEFE

- NFMp1 Optimise and investigate the photo-responsive properties and energy storage capabilities of azobenzene derivatives as MOST systems for energy generation and storage.
 NFMp2 Investigate norbornadiene derivatives as light harvesting and energy storing molecules for MOST systems.

DR T TSHIWAWA

- TTp1 Computational study of the inhibition of PCSK9.
 TTp2 Computational study of microRNA inhibition with anti-microRNA oligonucleotides.
 TTp3 Conformational study of alirocumab and evolocumab and their derivatives – the DFT approach

EM PROF G WATKINS

GMWp1 Nanomaterials: supramolecular structure from metal coordination with 1, 2, 4, 5-benzenetetracarboxylic acid and pyridine

• **DESCRIPTIONS OF RESEARCH PROJECTS 2025**

DR J BRITTON

JBp1 Modification of supercapacitor electrodes using carbon nanomaterials and phthalocyanines/porphyrins.

The rapid increase in global energy consumption and the environmental impact of traditional energy resources pose serious challenges to human health, energy security, and the environment; and reveal a growing need to develop new types of clean and sustainable energy conversion and storage systems.

Supercapacitors, or ultracapacitors, are energy storage devices that are considered “green” and are able to deliver their stored energy rapidly to whatever they are connected to. They can be used as a backup power source, in hybrid electric vehicles, for voltage smoothing and in a variety of other electronic devices.

Supercapacitors consist of two electrodes separated by an ion-permeable membrane, called a separator, and an electrolyte ionically connecting both electrodes. A supercapacitor stores electrical energy between two electrostatic double layers, which is created by forming thin charge layers on the interfaces of the electrolyte-electrodes.

Modification of the electrodes of a supercapacitor with different carbon nanomaterials, phthalocyanines and porphyrins could result in improved capacitance and other electrical properties of the supercapacitors. This is what will be investigated.

JBp2 Synthesis of ZnO and TiO₂ nanorod arrays for use in dye-sensitized solar cells in conjunction with phthalocyanines.

Nanowires (NW) are defined as metallic or semiconducting particles having a high aspect ratio, with cross-sectional diameters of about 1 μm, and lengths as long as tens of microns. Well-aligned one-dimensional nanowire arrays have been widely investigated as photoelectrodes for solar energy conversion because they provide direct electrical pathways ensuring the rapid collection of carriers generated throughout the device, as well as affording large junction areas and low reflectance owing to light scattering and trapping.

Solar energy conversion is a highly attractive process for clean and renewable power for the future. Excitonic solar cells (SCs), including organic and dye-sensitized solar cells (DSSC), appear to have significant potential as a low-cost alternative to conventional inorganic photovoltaic (PV) devices. The synthesis and application of nanostructures in solar cells have attracted much attention. Metal oxide nanowire (NW) arrays with large surface area and short diffusion length for minority carriers represent a new class of photoelectrode materials that hold great promise for photoelectrochemical (PEC) hydrogen generation applications. Up to now, various metal oxide nanostructures such as TiO₂, ZnO, Fe₂O₃, ZrO₂, Nb₂O₅, Al₂O₃ and CeO₂ have been successfully employed as photoelectrodes in SCs. Among the above-mentioned metal oxide nanostructures, the study of TiO₂ and ZnO is of particular interest due to the fact that they are the best candidates as photoelectrode used in SCs.

Phthalocyanines (Pcs) have also played a very important role in the development of DSSCs, as they are promising candidates for incorporation in these devices. Good efficiencies have been obtained by the use of

Pcs as the light harvester, and, most importantly, a number of synthetic strategies have been developed for engineered dyes based on the Pc scaffold, due to the synthetic versatility and robustness of these macrocycles.

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DR T GESWINDT

TGp1 The chemical origin of steam nano-bubbles

It has recently been reported that, when a low-concentration suspension of metal or carbon nano-particles dispersed in water is illuminated by sunlight, water vapour well above 100°C can be produced; with an overall energy efficiency of *ca* 24% and only a marginal heating of the bulk water.

This newly discovered direct conversion of sunlight into steam is sensational and has a tremendous potential as a game-changer for applications in process technology, solar fuels and various medical applications. However, the underlying physics and chemistry of this phenomenon is poorly understood – as it is expected that the emerging vapour would collapse and immediately condense upon contact with the surrounding colder liquid. Moreover, the dependency on the chemical composition of the aqueous solution certainly has an influence on the process efficacy, albeit hardly studied given the recent nature of this discovery.

In this research project, I would like to unravel the underlying chemistry and physics of this process by a combination of high-speed imaging, atomic force spectroscopy, Raman and related surface enhanced Raman spectroscopic methods (in collaboration with Stellenbosch University's Laser Physics group), ATR FT-IR spectroscopy, spectroscopic ellipsometry and theoretical modelling (DFT, TD-DFT, QM, MM). My working hypothesis is that the gas dissolved in the liquid plays an important role in the stabilization of the vapour bubble and the gas concentration will therefore be one of the crucial parameters to vary.

TGp2 Functionalization of polymeric supports with aliphatic (poly)amines in the use of PGM separation

It is known that (poly)amines illustrate selectivity toward the preferential separation of certain PGMs above others. The aim of this project is to functionalize silica (and subsequently polymeric supports) with selected amines in order to determine its efficacy in extraction of PGMs from industrial feed solutions.

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PROF R KLEIN

RKp1 Exploring Multicomponent reactions – an application of green chemistry principles

Multicomponent reactions are the combination of three or more molecules to give a final product in a one pot reaction. These types of reactions have the obvious advantage of achieving a target quickly and efficiently with fewer work up and purification steps, and in addition often demonstrate excellent atom economy, the use of catalytic methods and the potential to reduce energy use.[1]

We would like to use the Biginelli synthesis to develop a range of compounds with biological potential. The focus of this project will be to explore the possibilities of this reaction in producing differentially substituted dihydropyrimidones under mild conditions.

James E. Biggs-Houck, Ashkaan Younai, Jared T Shaw, Recent advances in multicomponent reactions for diversity-oriented synthesis, *Current Opinion in Chemical Biology*, Volume 14, Issue 3, 2010, Pages 371-382, ISSN 1367-5931, <http://dx.doi.org/10.1016/j.cbpa.2010.03.003>.

(<https://www.organic-chemistry.org/namedreactions/biginelli-reaction.shtml>)

RKp2 Catalysis

A chiral catalyst has been developed in our labs that is capable of catalysing a range of reactions. This project will look at making complexes using the new ligand system and a range of first row transition metals and test them in the aldol reaction and reduction reactions. If possible, we would like to grow crystals of one or more of these complexes.

RKp3 Green chemistry

We live in one of the most beautiful havens of biodiversity in the world! But we face the challenge of increasing our involvement in industrial chemistry in order to use our natural resources to promote jobs in order to grow our economy and support our population. We have the opportunity to do this in a sustainable way. This project will look at applying the principles of green chemistry to improving the synthesis a polymer using sugars as poly-ols. There will be catalysis, use of benign solvents and the application of many standard laboratory procedures.

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DR K Ramollo

KRp1 Synthesis and catalytic screening of transition-metal Schiff base complexes

Schiff base ligands are well renowned for their stabilizing effect when complexed to transition metals across the d-block. As such, the associated complexes have proven viable catalysts in both reduction and oxidation reactions, as well as a in a wide range of biological applications (such as antibacterial activity for example).

This project aims to synthesize a range of Schiff base ligands and associated late transition metal complexes for catalytic application in reduction reactions under homogeneous conditions. The ligands and complexes will be characterized by spectroscopic and spectrometric methods (such as NMR, FTIR, MS).

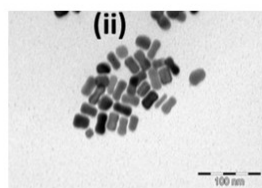
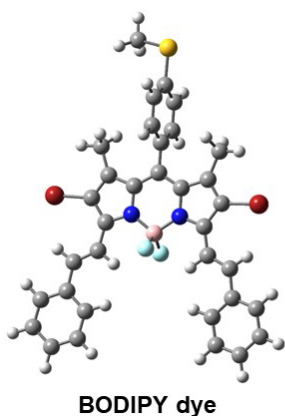
KRp2&3 Late transition metal Fischer carbene complexes as reduction catalysts (2 projects)

Traditional acyclic monoheteroatom-stabilized Fischer carbene complexes of catalytically relevant transition metals are underexplored. This project aims to synthesize novel Fischer carbene complexes of ruthenium. The isolated ruthenium complexes will be ascertained by NMR, FTIR, HRMS, and single crystal XRD characterisation techniques. The complexes will be screened as potential catalysts in the transfer hydrogenation of aryl ketones.

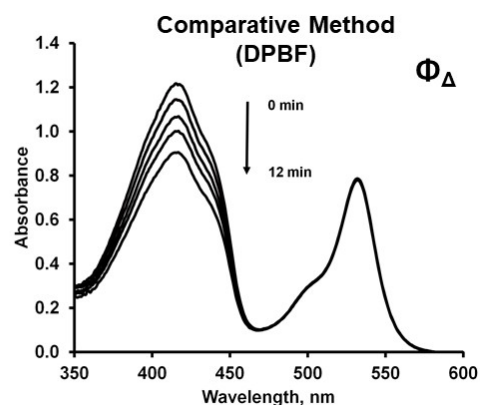
The second project will focus on the synthesis and characterization of iridium Fischer carbene complexes. As with the ruthenium project, the isolated iridium complexes will be fully characterized prior to catalytic screening in the arylation of selected aldehydes.

PROF J MACK

JMp1 Nanoparticle conjugates of BODIPY or azaBODIPY dyes for biomedical applications (Co-supervisor: Distinguished Prof. T. Nyokong)



Au nanoparticles

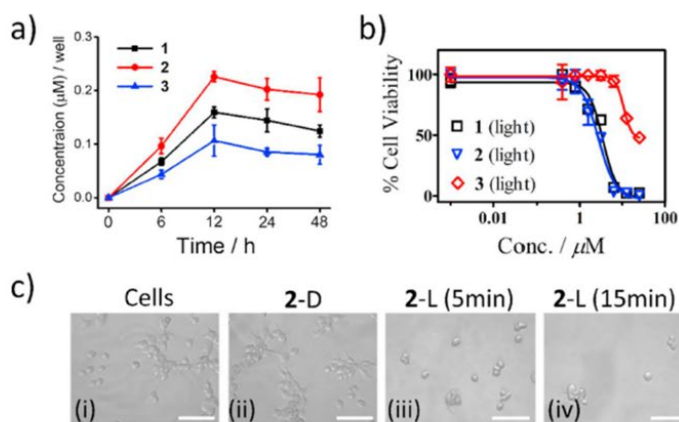
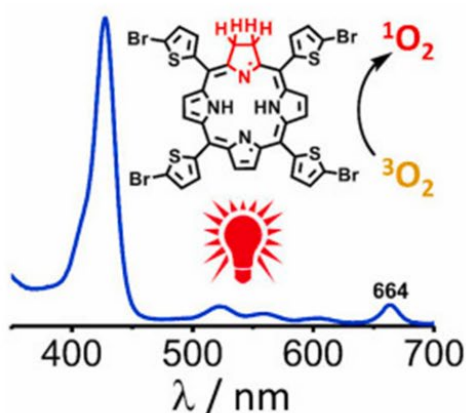


There is currently significant interest in the application of BODIPY and azaBODIPY dyes as photosensitizer dyes for photodynamic therapy (PDT). Although BODIPYs and azaBODIPYs normally have low triplet state quantum yields and absorb outside the therapeutic window, structural modification with heavy halogen atoms and styryl groups addresses these issues. The goal will be to conjugate novel BODIPY or azaBODIPY

dyes to gold nanoparticles for possible use as photosensitizers in PDT during the treatment of several different types of cancer. The project will involve the use of a laser flash photolysis system, the measurement of singlet oxygen quantum yields and *in vitro* PDT related studies with MCF-7 breast cancer cells.

References: H. Lu, J. Mack, Y. Yang, Z. Shen, Chem. Soc. Rev. **2014**, 43, 4778; R. C. Soy, B. Babu, J. Mack, T. Nyokong, Dyes Pigments **2021**, 194, 109631.

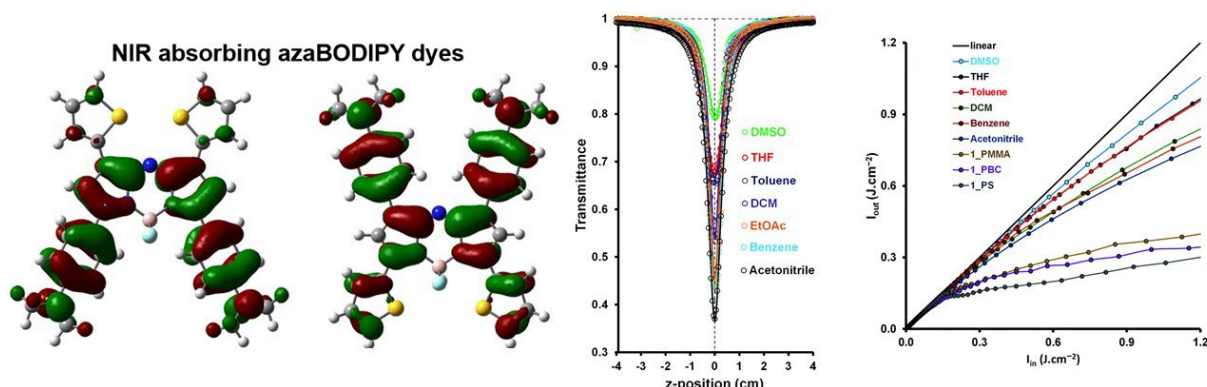
JMp2 Water-soluble porphyrin analogues for biomedical applications (Co-supervisor: Distinguished Prof. T. Nyokong)



There is considerable interest in the preparation of porphyrin analogues, such as octabromoporphyrins, chlorins and bacteriochlorins (with reduced peripheral pyrrole bonds), and N-confused porphyrins (with a pyrrole nitrogen on the periphery), that are water soluble, absorb and emit light at the red end of the visible region, and have high singlet oxygen quantum yields, since this makes them suitable for use as photosensitizers in biomedical applications such as photodynamic therapy (PDT) for the treatment of cancer. The project will involve the synthesis of a series of water-soluble porphyrin analogues, photophysical and laser flash photolysis measurements, and *in vitro* PDT related cell studies with MCF-7 breast cancer cells

References: J. Mack, Chem. Rev. **2017**, 117, 3444; B. Babu, A. Sindelo, J. Mack, T. Nyokong, Dyes Pigments **2021**, 185A, 108886; B. Babu, J. Mack, T. Nyokong, Dalton Trans. **2023**, 52, 5000.

JMp3 AzaBODIPYs for optical limiting of laser light (Co-supervisor: Distinguished Prof. T. Nyokong)



There is a growing problem in aviation safety related to the irresponsible use of laser pointers during the runway approach of aircraft and this has created a need for the development of optical limiting materials that can limit the transmission of high intensity laser pulses while remaining transparent under ambient light conditions. The goal of the project will be to prepare a series of near infrared absorbing azaBODIPY dyes and the preparation of azaBODIPY-embedded polymer thin films. Photophysical and non-linear optical

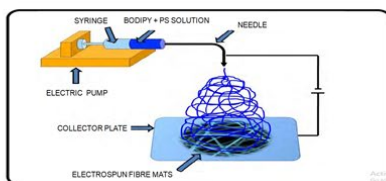
measurements will be performed to assess the suitability of the novel azaBODIPY compounds for optical limiting applications.

References: G. Kubheka, O. Achadu, J. Mack, T. Nyokong, *New J. Chem.* **2017**, 41, 12319; J. Mack, G. Kubheka, A. May, B. P. Ngoy, T. Nyokong, accepted by *Dalton Trans.* in **2024**. doi: 10.1039/D4DT02505A.

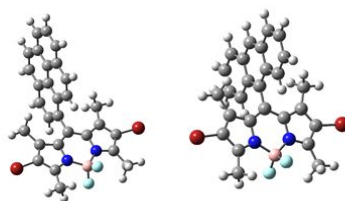
JMp4 **BODIPY-embedded nanofibres for wastewater treatment** (Co-supervisor: Distinguished Prof. T. Nyokong)



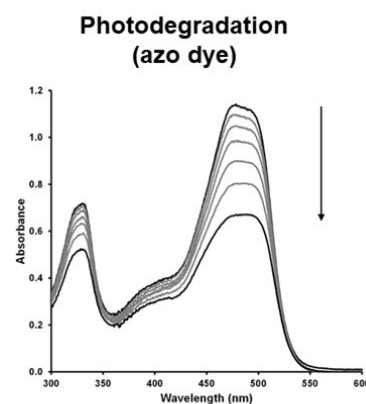
BODIPY embedded nanofibres



Nanofibre preparation



BODIPY dyes



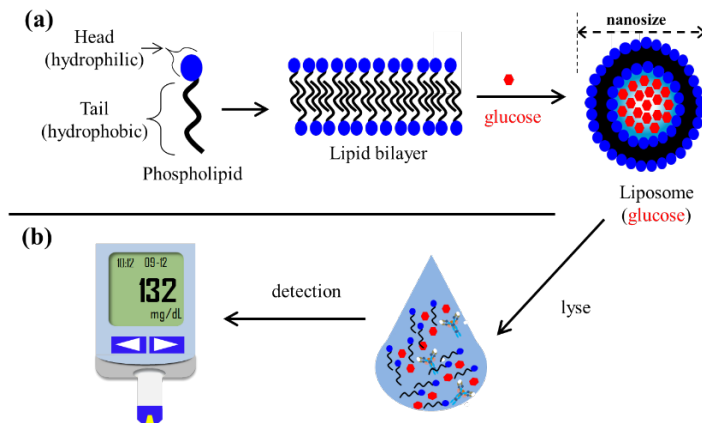
In recent years, halogenation has been used to significantly enhance the singlet oxygen quantum yields of BODIPY dyes. The high photostability of these dyes makes them ideal candidates for use in photodegradation applications, such as industrial wastewater remediation. The goal of the project will be to prepare a series of brominated and iodinated BODIPYs that can be conjugated to magnetic nanoparticles and to use electrospay polymerization to embed the nanoparticle conjugates into polystyrene nanofibers. The photophysical properties of the nanoparticle conjugates will then be investigated, and the suitability of the BODIPY-embedded nanofibers for use in the photodegradation of recalcitrant wastewater pollutants such as azo-dyes will be assessed.

Reference: A. K. Lebechi, T. Nyokong, J. Mack, *Macroheterocycles* **2017**, 10, 460.

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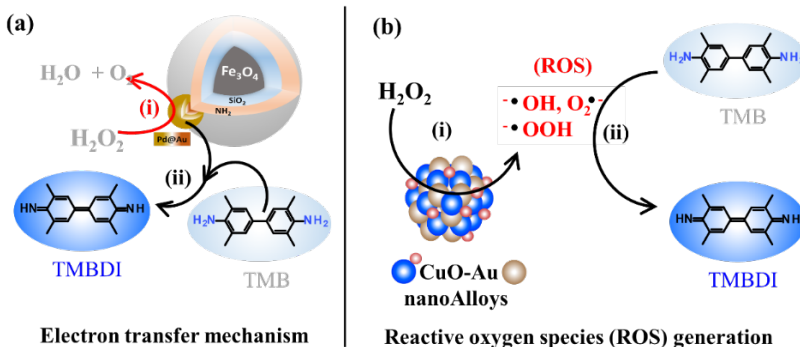
PNMp1 Preparation and characterization of pH-sensitive nanosize liposomes encapsulating D-glucose for electrochemical detection

The project will investigate methods for controlled preparation of pH-responsive liposomes loaded with D-glucose for electrochemical detection. The choice of the method for their preparation, the size control, optimum D-glucose encapsulation and the shelf-life (long-term stability) will be investigated. The research will also focus on the thorough characterization of these materials to obtain homogeneous sizes and determine the encapsulation efficiency. The formulation of these is of importance in achieving the pH response for the release of encapsulated glucose molecules. Scheme below shows the schematic representation of the preparation of liposomes.



PNMp2 Preparation and evaluation of enzymatic properties of nanomaterials core-shell and alloys

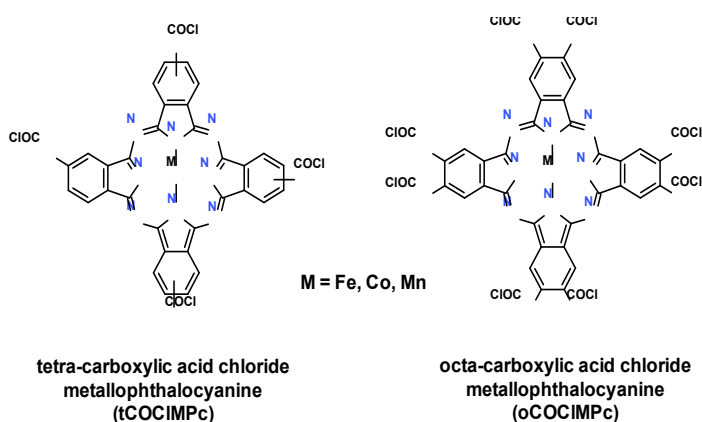
The research will investigate the preparation of size-controlled nanoparticles of bimetallic nanoparticles for their evaluation as nanozymes. The preparation method will determine whether the alloy or core-shell structure of nanomaterial formed. Studying the prepared nanomaterials as enzyme mimetic will involve determining their potential peroxidase or catalase-like properties. The preparation, characterization and evaluation of these materials is of importance as they could be use as substitutes for peroxidase or catalase enzymes in biochemical analysis. The scheme below shows some of the materials that have been investigated in my research group and that enzymatic mechanism were observed to be via (a) electron transfer or (b) reactive oxygen species (ROS) generation. The effect of nanomaterial composition will further elucidate the preference of either of the mechanisms.



PNMp3 Synthesis and spectroscopic characterization of tetra and octa-carboxylic acid chloride metallophthalocyanines and their thin monolayer films onto gold surfaces

Phthalocyanines, Pcs, are N-4 macrocycles that have been shown to exhibit numerous applications, such as in medicine as photosensitive drugs for the treatment of cancer, chemical industry as catalysts for photodegradation of pollutants, electrocatalysts for detecting molecules of research interest. Their applications are affected by the central metal ion within the phthalocyanine ring structure and by the functional groups on the peripheral and non-peripheral positions. The metal ions and functional groups also affect their spectroscopic as well as electrocatalytic properties.

In this research, metallophthalocyanines (MPc) containing peripheral acid chloride groups and electroactive central metal ions will be synthesized. These complexes will be immobilized onto gold electrode surface to form pH sensitive electrochemical sensors. The research will involve the synthesis and characterization of MPcs shown in the Figure below. Their immobilization onto gold electrode surface as monolayer thin films will also be investigated for the detection of neurotransmitters.



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PROFESSOR T NYOKONG

TNp1 Water purification using green technology (Co-supervised by Dr Britton– TWO projects).

The focus of this project is the use of nanotechnology combined with porphyrin-type dyes to develop materials that can provide solutions for water decontamination through advanced oxidation processes (AOPs). AOP uses molecular dioxygen and is an important strategy for pollution control, since it generally does not result in the formation of additional pollutants as by products [1]. AOP is considered as one of the most promising emerging green technologies for water treatment, due to the possibility of harnessing two readily available natural resources: dissolved oxygen and solar energy. Thus, the aim of the joint project is to link metallic and/or metal oxide nano/micro-particles to porphyrin-type complexes (Fig. 1) such as metallophthalocyanines (MPcs) and metalloporphyrins (MPs) to create new hybrid materials (Fig. 1, using ZnO as an example) for their intelligent use in environmental control.

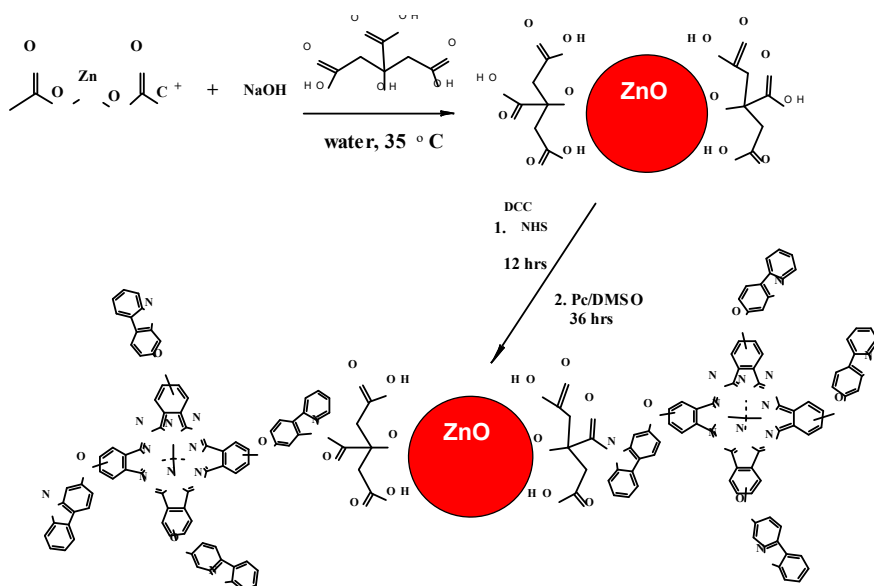
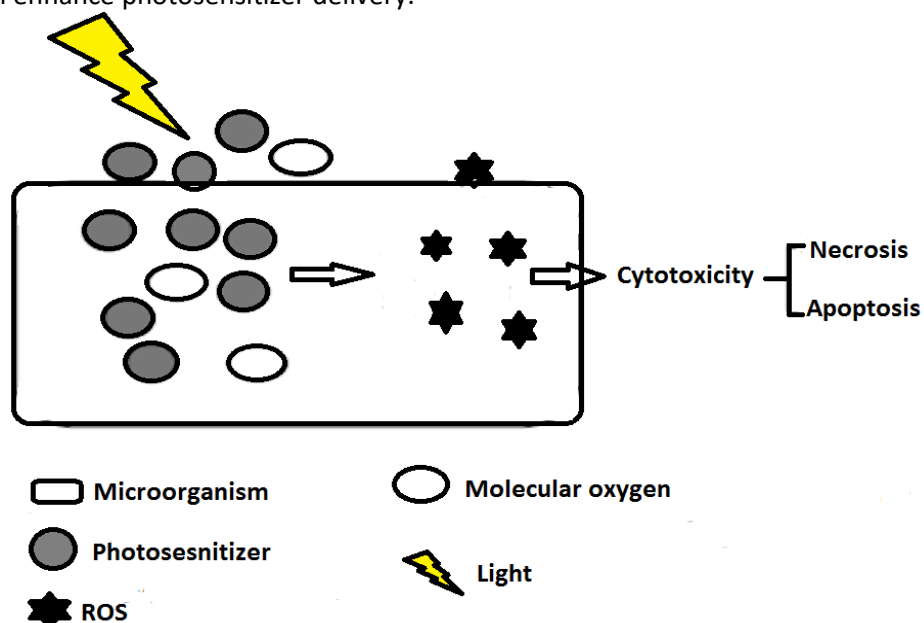


Fig. 1. Conjugation of nanoparticles to MPcs through an amide bond. DCC= dicyclohexylcarbodiimide, NHS = *N*-Hydroxysuccinimide, DMSO - dimethylsulfoxide

TNp2 Development of Antibacterial agents (Co-supervised by Dr Britton, TWO projects).

Antibiotics provide a remedy for microbial infections. However, in the past few decades, an increased number of drug resistant pathogens have been identified. The photoinactivation of microorganisms has been suggested as a means to avoid this problem. Photodynamic antimicrobial chemotherapy (PACT) is an alternative method to deal with bacterial and fungal infections, which requires a photosensitizer that can be illuminated with light to cause the oxidative destruction of microbial pathogens. The design of novel porphyrin – type complexes that have high singlet oxygen quantum yields is of great importance [2]. Many nanoparticles (NPs) such as plasmonic gold and silver NPs also exhibit antimicrobial behaviour and can be combined with porphyrin-type to form functional materials that will not only further enhance the PACT activity but will enhance photosensitizer delivery.



Scheme 1: Schematic diagram illustrating the principle of PACT [3].

For both projects 1 and 2, the porphyrin-type molecules and conjugates will be embedded in electrospun fibers for recovery and re-use. Electrospun nonwoven mats have a high surface area, small pore size, and high porosity. In this project, ZnO and TiO₂ nanofibers will be fabricated by electrospinning the solution of titanium or zinc compounds in the presence of polyvinylpyrrolidone (PVP). The ZnO/TiO₂ nanofibers will be decorated with MPCs following calcination with the aim of yielding regeneratable and possibly reusable catalysts. Since no catalytic activity is associated with the polymer and it merely acts as a support, calcination of the fibers not only yields purely crystalline fibers but also eliminates the possible shielding of the activity of the embedded catalysts by the polymer. Other fibers such as polystyrene containing porphyrin – type complexes will also be developed. The synthesis of the materials will be developed in parallel with the testing of the materials in applications related to organic/inorganic pollutant photodegradation and PACT.

TNp3 Protection of the eye and optical devices from strong laser light (Co-supervised by Drs Britton and Mack, TWO projects).

In recent years, the number of cases of pilots being exposed to laser, the so called "lasered" whilst landing aeroplanes has increased dramatically. Non-linear optical (NLO) devices that limit high incident power light (Fig. 2) has been proposed as a potential solution to these problems. Optical limiting (OL) is a specific branch of nonlinear optics and it refers to decreased transmittance of a material with increased incident light intensity.

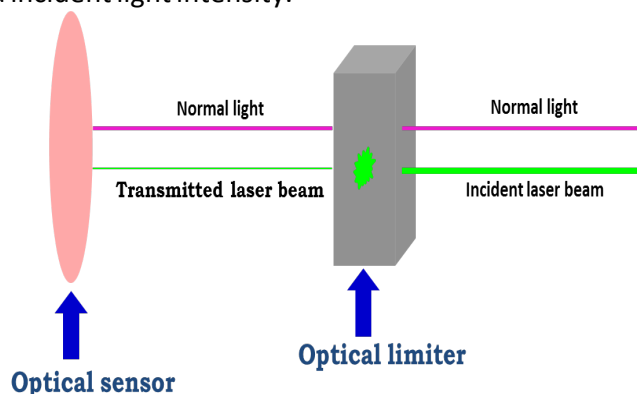


Fig. 2 Representation of optical limiting

There is a desperate and urgent need for materials which exhibit optical limiting capabilities and can prevent damage to the pilots' eyes and other optical devices. Phthalocyanines (Pcs) display nonlinear optical properties [3]. These molecules can thus be used for protection of optical elements (e.g. eyes) against damage by exposure to sudden high intensity light. OL is a nonlinear effect consisting of a decrease in the transmittance of NLO material (such as Pc) under high-intensity illumination. Phthalocyanines containing In and Ga as central metals exhibit good NLO properties and will be synthesized

1. P. Khoza, T. Nyokong, Visible light transformation of Rhodamine 6G using tetracarbazole zinc phthalocyanine when embedded in electrospun fibers and in the presence of ZnO and Ag particles, *J Coord Chem* 68(7) (2015) 1117-1131.
2. O. L Osifeko, I. Uddin, P. N. Mashazi, T. Nyokong, Physicochemical and Antimicrobial Photodynamic Therapy of unsymmetrical Indium phthalocyanines-Fe₃O₄-Silica core-shell conjugate, *New J Chem* 40 (2016) 2710 – 2721.
3. N. Nwaji, O. M. Bankole, J. Britton, T. Nyokong, Photophysical and Nonlinear Optical Study of Benzothiazole Substituted Phthalocyanine in Solution and Thin Film, *J. Porphyrins Phthalocyanines* 21 (2017) 263-272

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MRS J SEWRY

JSp1 Service-Learning: Working with the Mobile Science Laboratory

"Service-Learning is a method of teaching, learning and reflecting that combines academic classroom curriculum with meaningful service, frequently youth service, throughout the community"[http://en.wikkipedia.org/wiki/Service_learning]

The project entails assisting the Mobile Science Laboratory's team in designing curriculum-based practicals with pre- and post-lessons for Grade 10-12 learners. The researcher will take the pre- and post-lessons out to the schools two afternoons a term around the practical that the mobile science lab will run, and research the impact of the lessons and practicals. The practicals are aligned to the National Curriculum Statement and Assessment (CAPS). The researcher will also have to reflect on the work.

JSp2 Rhodes students' perceptions of tutoring at the Khanya Maths and Science Club

The Khanya Maths and Science Club is a RU Community Engagement project that runs maths tuition for grade 8 and 9 learners in Makhanda. The researcher will be doing a qualitative study, interviewing the tutors at the Khanya Maths and Science Club about their experiences as RU volunteers at the Club.

JSp3 What learning takes place during Chemistry 1 titration practicals?

The Chemistry 1 practical course requires students to do a number of titrations. It would be interesting to find out how much the students learn about chemistry in these practicals.

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DR V SMITH

VSp1 The reuse and repurposing of medicines through cocrystallization

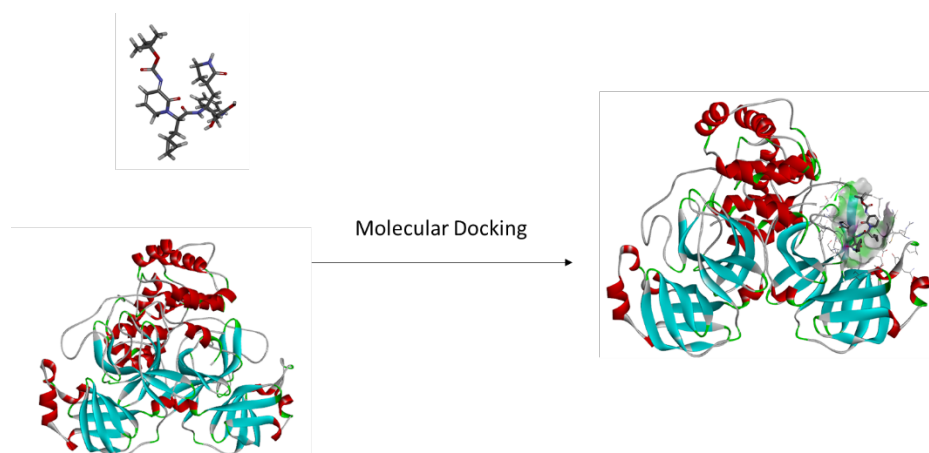
"Cocrystallization is a well-established technique used to repurpose and enhance existing active pharmaceutical ingredients by modifying their solid-state properties. This method, grounded in crystal engineering principles, is particularly effective in altering the physicochemical characteristics of compounds. By selecting appropriate pharmaceutically acceptable cofomers (partner molecules), cocrystallization can result in the formation of cocrystals that not only exhibit modified physicochemical properties but also demonstrate improved pharmacological efficacy." **Describe and discuss the many different ways to prepare and characterise cocrystals.**

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PROF KA LOBB

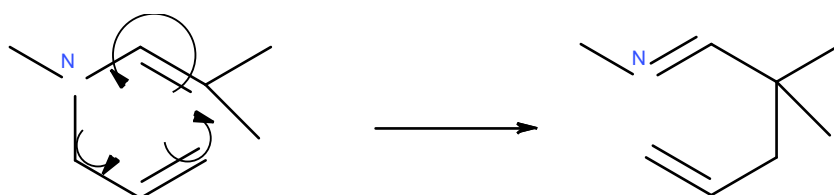
KALp1 Accurate prediction of ligand poses within protein active sites

Prediction of the pose of an inhibitor within the active site when complexed with a protein may be determined by experiment through x-ray crystallography or through NMR. However, there are several computational techniques that may be used to predict what will be found by experiment. In this project various computational tools will be used to perform molecular docking, and the resultant poses and interactions will be assessed so that the best pose is chosen. This will be compared to the experimental pose, to evaluate and improve upon the computational tool.

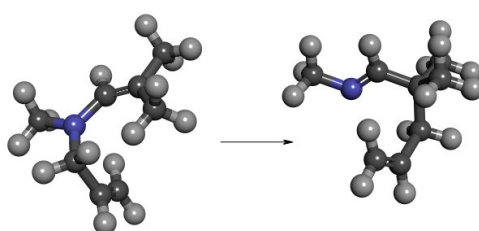


KALp2 Overview of the Aza-Cope rearrangement

The 3-aza-Cope rearrangement is a well-known reaction.



This is a computational project that will explore virtual compound databases and generate additional virtual libraries of compounds that are capable of undergoing variations of this type of rearrangement. From these models, a wide range of substrate, product and transition state geometries will be generated using computational techniques and the influence of substituent on the reaction energetics and on the intrinsic reaction coordinate (IRC) pathway will be explored.



DR NF MOLEFE

NFMp1 and NFMp2 The effect of the metal centre Cu and Zn on the properties of synthesised azobenzene liquid crystals.

Molecular solar thermal (MOST) systems are a more promising approach for harvesting and storing solar energy [1]. First proposed in the 1900s by Weigert: The concept is based on the idea that some molecules undergo a reversible photoswitching reaction between their conformers upon exposure to light [2]. This alters the molecular properties, such as geometry; thus, light energy is stored as chemical bonds [3]. Numerous molecules have been and are currently being studied for application as MOST systems due to their ability to act as photoswitches, which leads to processes such as isomerization, rearrangement, or dimerization of the molecule [1]. These molecules include anthracene, hydrazone, cubane, stilbene,

styrylpyrylium, **norbornadiene/quadricyclane** (NBD/QC), dihydroazulene/ vinylheptafulvene (DHA/VHF) couples, fulvalene dimetal complexes [FvRu₂(CO)₄], and azobenzene (AZBN) molecules, with the most promising being the NBD/QC, DHA/VHF, FvRu₂(CO)₄ complexes and the **trans-cis azobenzene** molecules [1–4].

However, examining how MOST systems work and finding critical requirements is necessary before introducing specific molecular structures and design solutions [1]. MOST systems must adhere to the energy storage cycle in four crucial processes (A–D) related to two fundamental quantities, ΔH^\ddagger and $\Delta H_{\text{storage}}$ (Figure 1).

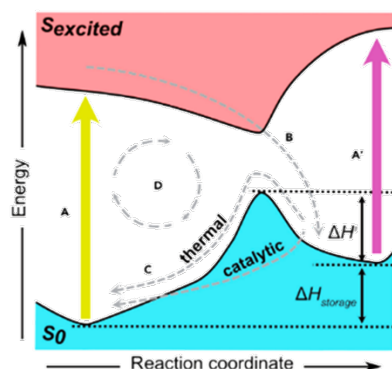
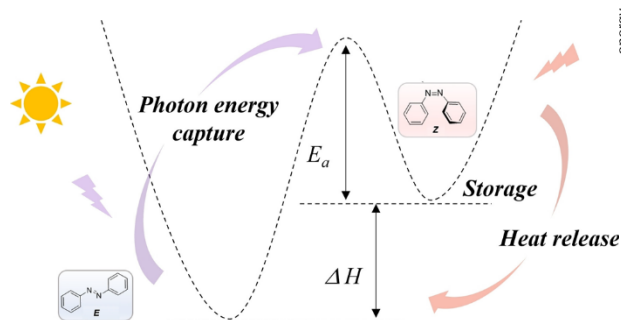


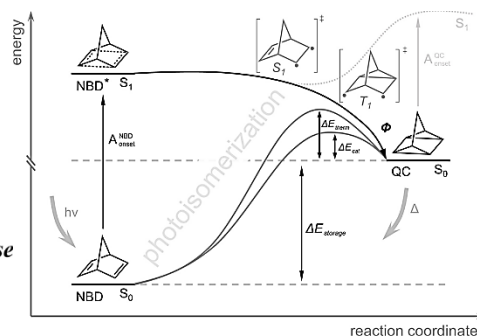
Figure 1: Illustration of the MOST system cycle, where S_0 to S_{excited} stands for the ground and excited conformer of the molecule, respectively. <https://doi.org/10.1016/j.joule.2021.11.001>

NFMp1



NFMp1: Multi-azobezene Photoswitches for Improved Molecular Solar Thermal Energy Storage, *Chem.Photo.Chem.*, Volume: 8, Issue: 8, First published: 15 March 2024, DOI: (10.1002/cptc.202400007)

NFMp2



NFMp2: The Norbornadiene/Quadricyclane Pair as Molecular Solar Thermal Energy Storage System, *Chem.Phys.Chem.*, Volume: 25, Issue: 9, First published: 20 February 2024, DOI: (10.1002/cphc.202300806)

- Hölzel H, Moth-Poulsen K. Molecular Solar Thermal Energy Storage Systems (MOST) -Design, Synthesis, and Application 2013.
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- Sun H, Tawa G, Wallqvist A. Classification of scaffold-hopping approaches 2013;17:310. <https://doi.org/10.1016/j.drudis.2011.10.024>.

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TTp1 Computational study of the inhibition of PCSK9 for the reduction of atherosclerotic cardiovascular disease

Over the years, cholesterol has earned a reputation as a high-risk factor for cardiovascular diseases. This is because the high concentrations of cholesterol in the blood may result in a build-up of plaque in the arteries that supply oxygen to the heart. Cholesterol build up in the arteries interferes with blood flow resulting in atherosclerotic cardiovascular diseases or a heart attack. Cholesterol is obtained by the body from dietary constituents, and many cells can synthesize their own endogenous cholesterol. Cholesterol in the blood is transported by lipoproteins (an assembly of proteins and lipids). Lipoproteins are classified based on their density, lipoproteins that consists of more lipids and less proteins are classified as low density lipoprotein (LDL), and lipoproteins that consists of less lipids and more proteins are classified as high density lipoproteins (HDL). This is because lipids have low density than proteins. LDL transport cholesterol to tissue cells, whereas HDL transports cholesterol from the tissue to the liver. Cholesterol in the liver may be used for a number of processes such as production of bile. The entry of cholesterol into the liver cells is facilitated by the LDL receptors (LDLR) on the liver cell membrane. PCSK9 protein binds to LDLR. When LDL binds to the PCSK9 bound LDLR, the complex is internalized into the lysosome where it is destroyed and LDLR is not recycled to the liver cell membrane and this will result in excess LDL cholesterol in the blood leading to atherosclerosis. Two PCSK9 inhibitors (alirocumab and evolocumab) were approved by the US Food and Drug Administration and European Medicines Agency. This study uses computational methods to elucidate the inhibitory pathways of alirocumab and evolocumab and search for cheaper drugs with better activity than evolocumab and alirocumab that target PCSK9. This study involves protein-protein docking and protein-ligand docking and subsequent molecular dynamics of the complexes.

TTp2 Computational study of microRNA inhibition with anti-microRNA oligonucleotides for cancer and cardiovascular disease treatment.

Several basic cellular activities such as transcription regulation, RNA processing and protein synthesis rely on nucleic acids interactions (RNA/DNA). In the cell there are small noncoding (about 20 nucleotides), double stranded RNA molecules called microRNAs that can mediate the expression of target genes with complementary sequence. Due to the importance of miRNAs in regulating cellular differentiation and proliferation, misregulation of miRNAs is linked to cancer and cardiovascular diseases. miRNAs can be inhibited by anti-microRNA (anti-miRNAs) that are single-stranded and chemically modified oligonucleotides. The inhibition of miRNAs is associated with therapeutic potential for cancer and cardiovascular diseases. This study involves the selection of aptamers (short, single-stranded DNA or RNA) with anticancer activities. Aptamers with affinity for a desired target are selected from a large oligonucleotide library through a process called SELEX. These aptamers will be docked to the miRNA through an RNA-RNA docking server and the complex will be put through a molecular dynamics simulation.

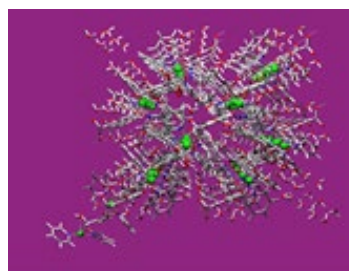
TTp3 Conformational study of alirocumab and evolocumab and their derivatives – the DFT approach

Alirocumab and evolocumab are PCSK9 inhibitors that were approved by the US Food and Drug Administration and European Medicines Agency for treatment against cardiovascular diseases in 2015. This study uses computational methods to generate derivatives of these two drugs and their subsequent conformational preferences. DFT calculations will be used to compute the properties of the molecular descriptors of such as the molecular orbitals and electrostatic potentials of the generated conformers from the derivatives of alirocumab and evolocumab.

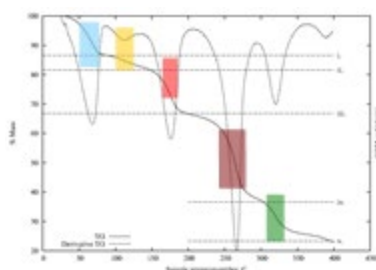
Return to [RESEARCH PROJECT \(SHORT TITLES\) 2025](#)

GMWp1Nanomaterials: supramolecular structure from metal coordination with 1, 2, 4, 5-benzenetetracarboxylic acid and pyridine:

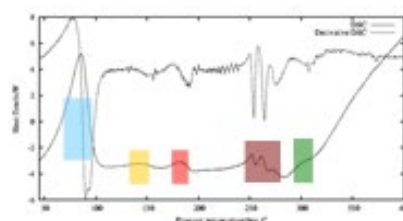
$\{[\text{Cu}_2 (\text{H}_2\text{C}_{10}\text{O}_8)(\text{C}_5\text{H}_5\text{N})_4(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}\}_n$ is a material with a bridge benzenetetracarboxylate frame work, 2 pyridines and axial H_2O bound to the copper. There is restricted channelling, containing 4 guest H_2O (z axis: cavity = $185 \text{ \AA}^3/\text{unit cell}$).



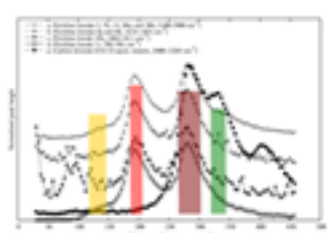
View down z axis



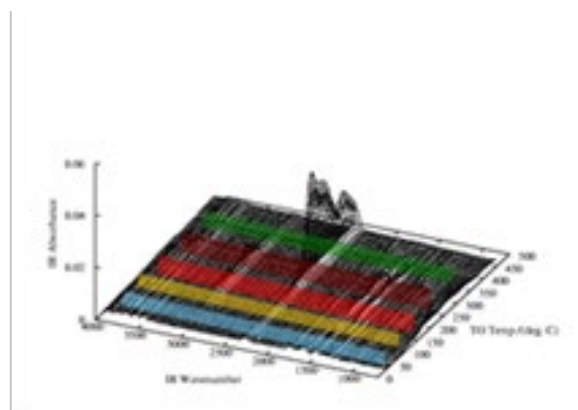
Thermogravimetric Analysis



Differential Scanning Calorimetry



Evolved Gas Analysis



The material undergoes loss of $6\text{H}_2\text{O}$ between 25 and 85 °C (blue: DSC - endotherm; TG - single step), loss of $\frac{1}{2}$ pyridine from 85 to 150 °C (yellow: DSC - endotherm; TG - broad step, EGA profile), loss of a further $1\frac{1}{2}$ pyridine from 150 to 197 °C (red : DSC - endotherm; TG - single step, EGA profile). Further heating causes decomposition, with rapid loss of loss of 2 pyridine, $1\frac{1}{2}\text{CO}_2$ and $1\text{H}_2\text{O}$ between 197 to 303 °C (brown: DSC – multistep endotherm; TG - broad step, EGA profile). Between 303 and 400 °C final loss of $\frac{1}{2}\text{CO}_2$ and 3CO occurs (green : DSC - endotherm; TG - single step, EGA profile). The thermolysis is shown in the time resolved stack plot.

Inclusion behavioural study of the material is limited by the need for exact thermal control. Below 85 °C inclusion of small solvent and gas molecules only is possible. The nature of the stable material formed between 150 and 197 °C ($[\text{Cu}_2 (\text{H}_2\text{C}_{10}\text{O}_8)(\text{C}_5\text{H}_5\text{N})_2]$) and its suitability to include guest molecules is to be investigated.

Synthesis of the 1st Transition Metal analogues (Mn to Zn) are to be explored and their thermal behaviour similarly investigated.

This project may make use of infrared and Raman spectroscopy, solid-state UV/VIS spectroscopy, TG-FTIR spectroscopy, thermal analysis, XRD, BET and XPS, amongst others.

PLEASE CHOOSE YOUR RESEARCH PROJECT AND ENTER YOUR CHOICES at

<https://docs.google.com/forms/d/1TvbQM3S5s824oRu4bYXWJK6MJnssaOKQ3gm8G19PHWQ/>

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9. THE REVIEW ESSAY (C)

Writing a review essay

In a review essay, the author is expected to synthesise information from a number of different sources, (in this case, research articles from journals) and show an understanding of what they have read. *No new information is presented.*

“A review essay is not a pure summary of the information you read for your review. You are required to analyze, synthesize, and interpret the information you read in some meaningful way.” (Bastek, 2021).

Outcomes for the review essay

Students should be able to (McKnelly, Morris, & Mang, 2021; Ogunsolu, Wang & Hanson, 2018;):

- Search for relevant literature (approx. five (minimum) or more research articles)
- Be able to read chemistry research articles
- Compile a list of references
- Narrow down information from a variety of sources
- Synthesise the information into an integrated document
- Learn to use a reference manager such as: Refworks, Mendeley, Zotero, InCites (see: <https://www.ru.ac.za/library/researchsupport/researchmanagementtools/> and the guide by Dr Goosen on RUConnected)
- Use Turnitin before submission of final draft for the purpose of checking your own use of sources and how much you have accurately and honestly made use of them.

The general structure of a review essay is as follows (Bastek, 2021):

- Title page
- Abstract (approx. 150 words; references are not included in the abstract)
- Introduction
- Discussion (divided into a number of topics or sub-topics)
- Conclusion
- References (Bibliography)

For the Chemistry Honours course:

Select an essay on a subject from the list supplied. The subject should not be directly related to the project. The Essay Supervisor must not be the same person as the project supervisor. The essay must be prepared in close consultation with the essay supervisor.

A first draft must be submitted by the end of the first term. The supervisor must record the dates when the FIRST and FINAL drafts of the essay were seen and approved. The first draft and the supervisor's comments must be handed in with the final draft to aid in the assessment of the candidate's contribution. The first and final drafts should preferably be submitted electronically, unless otherwise stated by the essay supervisor.

Students are required to submit their typed FINAL draft with their first draft by the end of the 2nd term. A Turnitin report must accompany the final report. The essay should be about 10 - 15 A4 pages (about 3000 words). At the end of the second term, each student will present a short seminar on their essay topic.

During the first three weeks of the Chemistry Honours course, students will:

- be given a key article by their essay supervisor
- visit the library and learn about search engines and reference managers
- attend a lecture/workshop on how to read a scientific article
- present a single slide on the key article, which must include (Ogunsolu, Wang & Hanson, 2018):
 - full reference of the article,
 - major topic(s) of the article,
 - the overarching theme
- Group the essay into topics and subtopics
- Do a peer-to-peer review of the topics and subtopics (McKnelly, et al, 2021)

By the end of the first term, students will submit a first draft of the essay to the supervisor.

Rubrics for the first (McKnelly, et al, 2021) and the final drafts are shown in Appendix III.

References

Bastek, N. (1994-2021). Review Essays for the Biological Sciences. The WAC Clearinghouse. Colorado State University. Available at <https://wac.colostate.edu/resources/writing/guides/>.

Ogunsolu, O. O., Wang, J. C., & Hanson, K. (2018). Writing a review article: a graduate level writing class. *Journal of Chemical Education*, 95(5), 810-816.

McKnelly, K. J., Morris, M. A., & Mang, S. A. (2021). Redesigning a "Writing for Chemists" Course Using Specifications Grading. *Journal of Chemical Education*, 98(4), 1201-1207.

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• REVIEW ESSAY TOPICS 2025

Dr J Britton

JBe1 Discuss how nanomaterials, phthalocyanines and porphyrins can be used in energy applications.

Dr T Geswindt

TGe1 The quantitative determination of pesticide residues on fruit (e.g. avocado) by means of LC-MS/MS and GC-MS/MS

Prof R Klein

RKe1 Teaching stereochemistry – methods and challenges

RKe2 Advantages and disadvantages of multicomponent reactions

DR K Ramollo

KRe1 Bonding modes of Schiff base ligands

Prof KA Lobb

KALe1 Applications of Car-Parrinello molecular dynamics

KALe2 Applications of semiempirical tight binding

KALe3 Theoretical prediction of NMR spectra

Prof J Mack

- JMe1 The synthesis, properties and applications of azaBODIPY dyes
- JMe2 Antibiotic resistance and photodynamic antimicrobial chemotherapy
- JMe3 Rational design of photosensitizer dyes for the treatment of cancer during photodynamic therapy
- JMe4 Dye-sensitized (Grätzel) solar cells
- JMe5 Theory and applications of MCD spectroscopy

Prof P Mashazi

- PNMe1 Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS): Principles, Data Acquisition and Analysis
- PNMe2 X-ray photoelectron spectroscopy (XPS): Data evaluation towards universal and standardised data analysis

Mrs J Sewry

- JSe1 Chemistry Security: History and Practices
- JSe2 Use of Chemometrics in a chemistry curriculum
- JSe3 The impact of ChatGPT and AI in Chemistry Education
- JSe4 The use of virtual laboratory in teaching practical skills

Dr V Smith

- VSe1 Discuss topics with Dr Smith.

Dr NF Molefe

- NFMe1 Effect of transition metals on liquid crystalline ligands.

Dr T Tshiwawa

- TTe1 The role of molecular modelling in the fourth Industrial Revolution.
- TTe2 The role of computational chemistry in green chemistry and sustainable development.

PLEASE CHOOSE YOUR ESSAY TOPIC AND ENTER YOUR CHOICES at
<https://docs.google.com/forms/d/1TvbQM3S5s824oRu4bYXWJK6MJnssaOKQ3gm8G19PHWQ/>

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10. APPENDIX I: COMMUNICATING CHEMISTRY

Writing a scientific report

As professional chemists, we (should!) record all of our experiments in lab books. But lab books are not very useful to other chemists who want to find out about our work. As a professional chemist, you will therefore need to write short reports summarising your work, and some fuller technical reports. The latter might take the form of:

- Honours project report
- MSc or PhD thesis
- Full research papers

Most full scientific reports cover these areas. The 1:2:3 guideline for length usually gives a well-balanced report, but is not always appropriate.

1. Introduction and background
2. Experimental details
3. Results and discussion
4. References
5. Summary or Abstract

[There may be additional brief sections]

• INTRODUCTION AND BACKGROUND

This is usually divided into three sub-sections:

- Brief summary of why the topic of the report is important/interesting
- Review of work in the area by others
- Statement of the specific aim(s) of the work

N.B. The introduction provides a general review of the topic - specific aspects of the work will require mini-reviews/references, as part of the 'Results & Discussion' section

• EXPERIMENTAL

This should report two things:

- a) A clear, concise description of what you did, so others can repeat it
 - b) An accurate record of your data, so others can confirm your interpretation.
- You usually report only the final experimental procedures in detail (e.g. optimised reaction conditions, final design of apparatus, and successful collection of data). How you arrived at these procedures will be discussed in the 'Results and Discussion' section, and the 'Experimental' section may contain a brief description of these other experiments.
 - You are strongly advised to follow the RSC format for presenting experimental details - see appropriate RSC journals.
 - It is a good idea to start writing up your 'Experimental' section in parallel with your lab research because:
 - i) It is quite time-consuming and fiddly, and can be a daunting job if left to the end.
 - ii) Writing up your 'Experimental' can help identify missing data or the need for extra experiments, and these can be dealt with immediately.
 - Check and double check the 'Experimental' section - these are your definitive results, so your scientific integrity is on show!

• RESULTS & DISCUSSION

- You need to be familiar with the work, and have worked out all of the key results.
- Schematically map out the story you will be telling, using headings/drawings/arrows.
- Use the scheme to produce headings and sub-headings for your report.

(Tip: These headings may remain in your final report (often very helpful to the reader, especially in long reports), or may simply provide guidance for the structure of your report (e.g. in a paper). In theses, the 'Results & Discussion' section may be divided into several chapters, to provide more clarity. Your story need not be chronological - look at all of your results, and decide how best to explain them to your reader).

- Write the story out in rough, referring extensively to tables, diagrams and schemes (yet to be drawn). The R&D section should summarise your experimental results, and provide brief confirmatory evidence that your interpretation is correct.
- Now draft out the graphics.
- Produce the final report in the correct format.

• SUMMARY (ABSTRACT)

Important - most reports must have a summary or abstract. Other scientists will often use the summary to help to decide whether to read a report/paper/thesis, and summaries often generate keywords that are used to locate important work. There is sometimes a specific format and length for summaries, but here is some advice:

- Decide the key results you want to report
- Identify three or four headings (e.g. aims, methods, key results, conclusion), and one or two graphics
- Use the headings to write a mini-story - it should be possible for a non-expert to read it in 3-4 minutes, and understand why you did the work, the main method(s) you used, the key results you obtained, and your principal conclusions

• REFERENCES

It is important that these are:

- Complete (don't miss any key papers)
- Accurate (get the citation right)
- Presented in a standard format

• ADDITIONAL SECTIONS

- **Keywords** are often required in papers, for cross-referencing in Chemical Abstracts or other databases, so others can find your work
- **Other layouts** are sometimes specified for scientific reports - e.g. Separate 'Results' and 'Discussion' sections
'Experimental Methods' section preceding 'Discussion'
- **Glossary** may be needed (e.g. abbreviations in a thesis)
- **Appendices** often contain useful additional data (e.g. NMR spectra, X-ray data, computer programs, equipment specifications)
- **Acknowledgments** - don't forget to thank everyone who helped with the work

11. APPENDIX II: COMMUNICATING CHEMISTRY

• GIVING AN ORAL PRESENTATION

You will almost certainly have to give many short talks during your career as a chemist. It may be just to a group of 5-6 colleagues at group meetings, or it may be to bigger audiences. However, you are the expert on your subject matter! You have done the experiments, or have read about your subject. So be confident, and don't go too fast or include too much detail. You must plan a talk that suits you (for style) and the audience (for clarity and interest) - just think about what the good and bad points are in lectures/talks you've attended. So here are some guidelines for a

20-minute chemistry talk, using PowerPoint presentation, there are also additional tips later in this section.

Planning

a) Divide your talk into 3 or 4 parts. Here is a common format, with approximate times suggested:

Introduction 3 min

Core (1 or 2 sections) 10 min

(Your results, or key points)

Summary or conclusion 2 min

Questions 5 min

b) Jot down what you want to say using:

- Snappy headings
- Brief sentences
- Structures
- Schemes
- Small tables/graphs/charts ... visual aids

c) Plan out about 6-8 slides

- Keep slides **simple**.
- Each slide will need to be up for **>1 min**.
- Structure your slides to help **guide** and **inform** your audience
- (N.B. slides can contain **prompts** for you).

Preparation

a) **Make up slides:**

- Use **big** drawings/type.
- Use **colour** for emphasis.
- **Check** that they are easily read at a distance.
- Have a good contrast between the background and the text

b) **Try the talk:**

- Just try **explaining** everything aloud, referring to your slides.
- If you're very nervous, write it all out **as a back-up, but do not read from your detailed notes**.
- Make **headings on a card** for reference.
- Possibly add something for **variety** (visual aid, anecdote).
- **Run through** the talk 3-4 times, ideally to a friend, until you're happy with content and length.

Giving your talk successfully

- Beforehand, check that you can work the projector/lighting etc.
- Try to stand relaxed, without fidgeting, and looking confident!

- Take it easy ... there's no rush ... refer to slides, but look at the audience as much as possible.

The end of the talk

- Try to finish on a high point (something successful).
- Make it clear you've finished - e.g.
"Thank you for your attention" (not "That's it!")

After your talk

- Get some feedback - you need an honest friend to tell you the best things about your talk and also the features that were less successful.

Some additional tips:

Preparation

- Using composite slides (where you add or reveal information to gradually generate a complex slide) works well.
- Mixed media presentations (e.g. slides + demonstration + video projector) are great, but lots of quick changes between different media can bewilder an audience

Giving your talk

- If you are offered a microphone in a large room, use it
- Maybe write out your first sentence ... but make yourself use card headings thereafter
- Look at the audience ... although just over their heads has the same effect!
- Try not to block your audience's view of the screen - if you want to point to something on a slide, simply point a laser point at the appropriate bit of the slide.
- If you stumble over your words, or spot any mistakes on your slides, just carry on regardless ... like any other performer would!

At the end

- If questions are asked, take your time to answer, and admit if you don't know. One good tactic is to repeat the question in your own words, which:
- Ensures everyone can hear the question
- Means it is clear what question you'll answer and buys you a bit of time to think of an answer!

12. APPENDIX III: ASSESSMENT RUBRICS for the essay and project

Marking rubric for FIRST draft of essay (McKnelly, et al, 2021)

Rubric criteria		Met	Not met
Sentence level	Writing is grammatically correct		
	Words are spelt and used correctly		
	Sentences are constructed correctly		
Paragraph level	Each paragraph has a clear and coherent topic sentence		
	“Each paragraph has one clear and coherent main idea that relates to the thesis of the piece of writing”		
	The order and flow of paragraphs is clear and logical		
Essay level	The intended audience is clearly addressed		
	The topic of the essay is supported by the rest of the essay		
	“All assertions are supported with evidence”		
	“The writer has constructed a consistent and coherent narrative”		
Very good: 8/10			
Satisfactory: 6/10			
Unsatisfactory:			

Marking rubric for FINAL draft of essay

Student Surname, Initials _____

Student number _____

Criteria	Highly competent	Competent	Does not meet minimum criteria	Unacceptable	
Abstract	Contains the essence of the essay and written well (5)	A good summary of the essay (3-4)	A fair reflection of what the essay is about (2)	Reader has no idea what the essay is about (0-1)	5
Content	Sufficient, relevant, accurate and appropriate; a detailed presentation with no errors. (51-65)	Good evidence on relevance and accuracy but weaker on sufficiency and appropriateness (minor errors) (31-50)	Dubious relevance and inaccuracy on key points; significant numbers of errors. (16-30)	Limited relevance and serious inaccuracy reflected in large number of errors. (0-15)	65
Conceptual coherence	Different subtopics dealt with under different subheadings; flows well. Content well directed to answering question and presenting cohesive discussion. Central argument clear, well supported by literature as evidence. (8-10)	Evidence of differentiation and some planning; some logical flow in the construction of a central argument. Appropriate use of literature as evidence. (5-7)	Limited conceptual cohesion, rather a collation of unrelated pieces of information related to the topic. Inadequate use of literature as evidence. (3-4)	No coherence, only part of the information related to the question is provided. Little or no organization towards a central argument. Inappropriate or inadequate use of literature. (0-2)	10
Organization	Well organized and planned, ideas and concepts flow logically (8-10)	Reasonable outline. Most of work well-directed towards	Little evidence of planning and no clear	No evidence of planning. (0-2)	10

		central argument with some loose ends essentially unrelated. (5-7)	links between how sections build towards a conclusion. (3-4)		
Presentation	Neat with no grammar/ spelling mistakes (5)	Neat with few grammar/ spelling mistakes (3-4)	Numerous spelling/ grammar errors (2)	Untyped work, lack of proofreading (0-1)	5
References	All claims are referenced; reference list complete; Consistency in citations and references; Evidence of reference manager used (5)	Most claims are cited; some inconsistencies in the list of references; reference manager has been used (3-4)	Few claims are referenced, poorly constructed reference list; no reference manager (1)	No citations; no references, no reference manger (0)	5

Assessed by: _____

Date: _____

Final mark/100 _____

Moderated by: _____

Date: _____

Final mark/100 _____

Project evaluation grid

Student Details		
Student Name		
Project Title		
	Rating	Motivation (i.e. Comments)
Personal (20%)	/20	/20
Attitude and Initiative (10)		
Research Aptitude (10)		
The Project (30%)	/30	
Were the goals achieved? (5)		
Difficulty of the problem (5)		
Initiative and problem-solving ability (10)		
Lab Notebook (10)		
The Report (50%)	/50	
Layout (5)		
Grammar and spelling (5)		
Abstract (5) (clear)		
Introduction (5) (A literature review, Aims and Objectives)		
Results and Discussion (10) (Not just a list of results; Interpretation of data)		
Conclusion (5) (Were the objectives achieved; If not, why not?)		
Experimental (10)		

(Clear, can be repeated)		
Referencing (5) (Uniform, Standard)		
Overall Mark		
Summary		

13. APPENDIX IV: Plagiarism form

(to be completed and handed to Chemistry Administration office)



RHODES UNIVERSITY
Where leaders learn

Department of Chemistry

Surname and initials: _____ Student No: _____

DECLARATION

1. I have read the University Policy on Plagiarism and am aware of the possible consequences of plagiarism
https://www.ru.ac.za/media/rhodesuniversity/content/institutionalplanning/documents/policies/Common_Faculty_Policy_and_Procedures_on_Plagiarism.pdf
2. I know that “plagiarism” means using another person’s work and ideas without acknowledgement, and pretending that it is one’s own. I know that plagiarism not only includes verbatim copying, but also the extensive (albeit paraphrased) use of another person’s ideas without acknowledgement. I know that plagiarism covers this sort of use of material found in textbooks, journal articles, theses AND on the internet.
3. I acknowledge and understand that plagiarism is wrong, and that it constitutes academic theft.
4. All submitted work is my own work, or the unique work of a group, if a group assignment.
5. I will not allow anyone to copy my work with the intention of passing it off as their own work. I also accept that submitting identical work to someone else (a syndicate essay) constitutes a form of plagiarism.
6. I acknowledge that using anything from the internet, without referencing it correctly is a form of plagiarism. I will NOT make use of any website that gives me the answer to a problem/assignment/essay/tutorial or any other form of assessment.

Signed _____ Date _____

14. CHOICE FORMS

The FINAL CHOICE FORM will be completed during the *FIRST WEEK* of the Honours Course via a Google form. Details will be given during the first week of class.

The form below can be used to jot down what you would like to do.

CHOICE INDICATION

Circle the **FIFTEEN** lecture topics likely to be chosen by you, fill in details of your essay (first, second, and third choices) and project (first, second, and third choices).

LECTURE TOPICS:

PAPER 1:	VS1	PNM1	GW2	NFM2	RK3	KR1		
PAPER 2:	TT1	JM2	PNM2	NFM3	RK1	TG2		
PAPER 3:	JS1	EA1	KAL1	JM3	GW1	VS2		
Cont. Assess.	VL1	KAL3	JS2	JM1	TT2	TG1	RK2*	

* compulsory, but not for examination purposes

PROJECT: (SHORT TITLE)

INITIALS

1st Choice:

Supervisor:

2nd Choice:

Supervisor:

3rd Choice:

Supervisor:

ESSAY: (NUMBER) [make sure you choose a DIFFERENT supervisor here]

1st Choice:

Supervisor:

2nd Choice:

Supervisor:

3rd Choice:

Supervisor: