

**QUALITY ASSURANCE MANUAL  
DEPARTMENT OF BIOCHEMISTRY AND MICROBIOLOGY**

<b>MSc PROGRAMME OUTLINE</b>		
<b>MSc in Bioinformatics and Computational Molecular Biology</b>		
<b>Course Work / Project Masters</b>	<b>Year: 2021</b>	<b>Coordinators: Prof Özlem Tastan Bishop &amp; Mrs Stacey Glenister</b>

**COURSE WORK and RESEARCH THESIS MASTERS**

**in**

**BIOINFORMATICS and  
COMPUTATIONAL MOLECULAR BIOLOGY**

**2021**

**DEPARTMENTS**

**of**

**BIOCHEMISTRY & MICROBIOLOGY,  
CHEMISTRY, MATHEMATICS AND STATISTICS**

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**ORIENTATION**

**(1 March 2021, Monday)**

**(Place: Online via Zoom, links will follow)**

09:30 – 10:00	Welcoming and introduction of RUBi members
10:00 – 10:30	Introduction to the programme
10:30 – 11:00	Introduction to plagiarism

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**PROPOSED PROGRAMME FOR 2020**

Date	Module	Content
2 <b>March</b> , Tues - 5 <b>March</b> , Fri  [20 hours]	<b>Introduction to Linux</b>  Dr Allan Sanyanga	Linux operating system and software installation; Use of Linux and Linux shell commands; Introduction to Bash and Bash scripting; Applications to Bioinformatics problems.
8 <b>March</b> , Mon – 1 <b>April</b> , Thu  [80 hours] 22 March – P/H	<b>Python for Bioinformatics</b>  Dr Allan Sanyanga	Introductory and advanced Python; HPC cluster.
2 <b>April</b> , Fri, 5 <b>April</b> , Mon	<b>Easter Holiday</b>	
6 <b>April</b> , Tues - 9 <b>April</b> , Fri	<b>Python assignment week</b>  Dr Allan Sanyanga	
12 <b>April</b> , Mon - 16 <b>April</b> , Fri  [25 hours]	<b>Basic Genomics</b>  Prof Özlem Tastan Bishop	Biological databases; Data retrieval; Sequence alignment and visualization.
19 <b>April</b> , Mon – 23 <b>April</b> , Fri  [25 hours]	<b>Structural Bioinformatics I</b>  Prof Özlem Tastan Bishop	Introduction to structural biology; Homology modeling and model validation.

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26 April, Mon – 30 April, Fri	<b>Study/revision week, Start of projects</b>	
3 May, Mon - 7 May, Fri	<b>EXAMINATIONS:</b> <ul style="list-style-type: none"> <li><b>Linux</b> (3 May)</li> <li><b>Basic genomics</b> (4 May)</li> <li><b>Python</b> (6 May)</li> <li><b>Structural Bioinformatics</b> (7 May)</li> </ul>	
10 May, Mon - 14 May, Fri  [25 hours]	<b>Structural Bioinformatics II</b>  Prof Kevin Lobb	Computational chemistry levels of theory. Protein-small molecule interactions; Ligand docking programs.
17 May, Mon - 21 May, Fri  [25 hours]	<b>Structural Bioinformatics III</b>  Dr Vuyani Moses	Molecular dynamics simulations of protein-ligand complexes.
24 May, Mon - 28 May, Fri  [25 hours]	<b>Structural Bioinformatics IV</b>  Dr Vuyani Moses	Force field parameter evaluation.

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7 <b>June</b> , Mon - 11 <b>June</b> , Fri	<b>Study/revision week</b>	
14 <b>June</b> , Mon - 17 <b>June</b> , Fri  [25 hours]	Matlab and Artificial Neural Networks  Prof Nigel Bishop	Review of basic <b>Calculus</b> and linear algebra; Mathematical programming using the MATLAB computational environment. Use of artificial neural networks in MATLAB.
21 <b>June</b> , Mon - 23 <b>June</b> , Wed  [15 hours]	<b>Statistic</b>  Mr Jeremy Baxter	Introductory statistics; R: statistical software.
	<b>EXAMINATIONS:</b> <ul style="list-style-type: none"> <li><b>Structural Bioinformatics II</b> (25 June)</li> <li><b>Structural Bioinformatics III</b> (28 June)</li> <li><b>Structural Bioinformatics IV</b> (29 June)</li> <li><b>Statistics</b> (30 June)</li> <li><b>Matlab and Artificial Neural Networks</b> (1 July)</li> </ul>	
2 <b>July</b> , Tue -11 <b>July</b> , Sun	<b>BREAK</b>	
12 <b>July</b> , Mon	<b>Project starts!</b>	
26 <b>July</b> , Mon	<b>PROJECTS:</b> Hand-in Literature Review and Project Proposal to Supervisor and Co-supervisor	
26 <b>July</b> , Mon - 30 <b>July</b> , Fri	<b>PROJECTS:</b> Project Proposal Presentations	
23 <b>August</b> , Mon - 27 <b>August</b> , Fri	1 <sup>st</sup> Presentation of Project Progress	

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<b>4 October, Mon - 8 October, Fri</b>	<b>2<sup>nd</sup> Presentation of Project Progress</b>
<b>22 November, Mon - 26 November, Fri</b>	<b>Presentation of project results</b>
<b>6-13 December</b>	<b>Thesis submission (If thesis on time)</b>

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**OVERALL TEACHING HOURS**

	<b>Contact Hours</b>	<b>Lecturing Hours</b>	<b>Practicals and tutorials</b>
<b>Introduction to Linux</b>	20	10	15
<b>Basic Genomics</b>	25	10	15
<b>Python for Bioinformatics</b>	80	32	48
<b>Structural Bioinformatics I</b>	25	10	15
<b>Structural Bioinformatics II</b>	25	10	15
<b>Structural Bioinformatics III</b>	25	10	15
<b>Structural Bioinformatics IV</b>	25	10	15
<b>Statistics</b>	15	10	5
<b>Mathematics and MATLAB</b>	25	10	15
<b>TOTAL</b>	<b>265</b>	<b>112</b>	<b>82</b>



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## **COURSE OUTCOMES**

### **CRITICAL OUTCOMES ADDRESSED**

1. Identify and solve problems and make decisions using critical and creative thinking
2. Work effectively with others as a team
3. Organise and manage time and activities effectively
4. Collect, analyse, organise, and critically evaluate information
5. Communicate effectively using written, electronic and language skills
6. Use science and technology effectively and critically showing responsibility towards the environment and others
7. Demonstrate an understanding of the world as a set of related systems

### **SPECIFIC OUTCOMES ADDRESSED:**

1. Develop a broad understanding of what the field of Bioinformatics and Computational Molecular Biology comprises
2. Develop an in-depth knowledge of certain major areas of Bioinformatics and Computational Molecular Biology
3. Demonstrate the ability to conduct research by designing and carrying out a piece of research in Bioinformatics and Computational Molecular Biology, including design of computational experiments and collection and analysis of data
4. Demonstrate expertise in scientific writing, oral presentation and communication
5. Demonstrate an understanding of the relationship between Bioinformatics and Computational Molecular Biology, the community and the environment
6. Demonstrate the competence required for recognition as a professional Bioinformaticist or Computational Molecular Biologist in South Africa
7. Develop professional attitudes and values including scientific ethics and integrity

### **PARTICULAR SKILLS TO BE ACQUIRED:**

1. Scientific communication and presentation skills including computer skills
2. Ability to use the scientific literature efficiently and effectively
3. Practical skills required for use and application of computers and software
4. Organisational skills required to acquire, manage and utilise data and information
5. Ability to analyse and evaluate scientific data
6. Good computer practice

### **GENERAL BACKGROUND & OUTCOMES**

Bioinformatics and computational molecular biology is the systematic development and application of information technologies and data mining techniques for analysing biological data obtained by experiments, modelling, database searching and instrumentation to make novel observations and predictions about biological function. This course will be taught in an interdisciplinary manner and focussing on the interface between the computational sciences and the biological, physical and chemical sciences. Graduates who complete this course will

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be skilled in the assimilation of biological information through the use and development of computational tools for a range of applications including simple pattern recognition, molecular modelling for the prediction of structure and function, gene discovery and drug target discovery, the analysis of phylogenetic relationships, whole genome analysis and the comparison of genetic organization.

**COURSE STRUCTURE, TEACHING METHODS & APPROACH**

The Masters programme will be offered over 11 months and incorporate a number of course work modules and a research project running concurrently throughout the programme. The course work modules will involve an integration of formal lectures, self-learning computer-based tutorials and practicals. In addition, problem solving tutorials would be designed to guide the student through current information-based problems and involve the assimilation and reduction of biological information. A number of the tutorials and practical components will be assessed and contribute towards a course work year mark. The assessment of the course work component would be through assignments, tutorials, tests etc., and examinations. Each examination will have an external examiner, appointed by the lecturer's home Department (for lecturers from Rhodes), or by the Department of Biochemistry, Biotechnology and Microbiology (for external lecturers).

The research projects will be computer based. The projects will be assessed by seminar presentations of the proposed and final work, and by a written thesis. Each thesis will be examined by two external examiners.

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**ASSESSMENT**

**OVERALL**

The course-work and the research work will each contribute 50% to an overall mark. Successful completion of the course will be subject to a final mark of at least 50%, provided that a candidate obtains at least 50% for the course work, with a sub-minimum of at least 40% from each module, and at least 50% for the project report.

**COURSE WORK**

The course-work modules will be assessed by internal grading of tutorials, assignments, tests and practicals, etc. to give a class mark; and by internal and external grading of examinations. The calculation of the class mark for each module is given later in this manual under the detailed entry for the module. The examinations will be given during the period specified in the course programme earlier in this manual. For each module, the weighting between class mark and examination towards the module mark will be

- Class mark                      40%
- Examinations                    60%

The weightings of the various modules in the calculation of the overall course work mark will be proportional to the number of lectures given. For each module the weighting, and the duration of the examination, will be

<b>Module</b>	<b>Weighting</b>	<b>Duration (hours – up to)</b>
Introduction to Linux	7.2%	3
Basic Genomics	9.1%	3
Python for Bioinformatics	29.1%	4-5
Structural Bioinformatics I	9.1%	3
Structural Bioinformatics II	9.1%	3
Structural Bioinformatics III	9.1%	3
Data structures & algorithm	9.1%	3
Statistics	9.1%	3
MATLAB	9.1%	3

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### **PROJECT**

The project will be graded internally and externally with the following weightings:

- Project proposal and presentation 10%
- Project results and presentations 30%
- Thesis 60%

### **PROPOSAL:**

#### **Guidelines**

Preparation for the Research Project Proposal (written and oral) should be commenced as soon as the projects have been allocated.

#### *Written*

**Style:** Follow the style of any journal article on Bioinformatics

**Length:** Around 20 typed pages. Include sections on: Literature review (around 15 pgs); problem statement and hypothesis (1 pg); aims and objectives (1 page); outline of approach and methodology (1–2 pgs).

**References:** Follow the citation and listing style of the journal, (references may be single-spaced).

#### *Oral*

**Length:** 30 minutes; 25 minutes presentation and 5 minutes questions.

#### **Dates**

As specified in the programme earlier in this manual.

#### **Marks Breakdown**

- Proposal presentation: 50%
- Written proposal: 50%

### **PRESENTATION OF PROJECT RESULTS:**

#### **Guidelines**

The Research Project Results presentation should include:

- **Introduction** - an explanation of the background to the project, the current status of the scientific field, a clear hypothesis statement, and the overall aims & objectives of the project.
- **Description of the approach**, the techniques and methodology, including reasons for why these computations were done.

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- **Presentation and Explanation of Results.**
- **Critical discussion of results** including analysis of their implications, and any problem areas.
- **Conclusion** that includes the overall outcome of the project and where future research should be directed.

**Dates**

As specified in the programme earlier in this manual.

**THESIS:**

**Structure**

There is some flexibility in the choice of format for a thesis, but as a guide, it should contain the following sections in the order given:

Abstract  
Table of Contents  
Table of Figures  
List of Tables  
List of Abbreviations  
Acknowledgements  
Chapters 1 (Literature review)  
Chapter 2, 3, etc  
Conclusion  
References

Each Chapter following Chapter 1 would normally contain

Introduction  
Methods  
Results and Discussion

**Dates**

As specified in the programme earlier in this manual.

**ASSESSMENT CRITERIA & PROCEDURE**

The thesis will be assessed by two external examiners. Preferably, at least one of the external examiners should be international.

**NUMBER OF COPIES OF THE RESEARCH REPORT**

You should prepare two copies of your thesis for external examiners. After corrections are done, one final copy should be prepared for RUBi.

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**DESCRIPTION OF THE MAJOR SECTIONS OF THE THESIS**

**1. ABSTRACT**

An abstract has to stand alone and should: (i) state the principal objectives and scope of the investigation; (ii) state the methodology used; (iii) summarize the results; (iv) state the principal conclusions. It should not exceed a page.

**2. CHAPTER 1**

**Literature review**

This should be a concise summary that describes the current status of the research field. It should be current and comprehensive.

**Project aims, objectives and motivation**

A clear statement of the aims & objectives of the project and motivation for these should be given. Knowledge gap should be explained.

**3. FURTHER CHAPTERS**

**Introduction**

This should be a concise summary that describes the current status of the literature related to the chapter.

**Methodology**

This should give a logical account of the methodology. It should be precise and complete.

**Results and Conclusion**

This section should give a description of the results of the experiments together with an explanation of why they were done. It should include critical analysis of the data and interpretation of the implications of the results.

**4. CONCLUSION**

Should be a concise and relevant summary, including the contribution the research makes to the current status of the field. A statement of the direction of future research arising from the project should be given.

**5. REFERENCES**

Current research articles should be used and cited in the text of the thesis using the style of a bioinformatics journal.

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**EVALUATION FORMS**

**MSc Proposal Presentation Evaluation Criteria**

<b>Criterion</b>	<b>Weight</b>
1. Concise, accurate & up-to-date literature review	<b>20</b>
2. Knowledge gap and/or problem clearly identified and stated	<b>20</b>
3. Clear research hypothesis & objectives; Concise description of approach and methods	<b>20</b>
4. Research objectives, approach & methods. Realistic? Feasible?	<b>15</b>
5. Time management, visual media and speaker – audience contact	<b>10</b>
6. Ability of speaker to answer questions in a clear & meaningful manner.	<b>15</b>

**MSc Written Proposal Evaluation Form**

<b>Criterion</b>	<b>Weight</b>
1. Concise, accurate & up-to-date literature review	<b>30</b>
2. Knowledge gap and/or problem clearly identified and stated	<b>20</b>
3. Clear research hypothesis & objectives; Concise description of approach and methods	<b>20</b>
4. Research objectives, approach & methods. Realistic? Feasible?	<b>15</b>
5. Quality of scientific writing	<b>15</b>

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**MSc Project Progress Presentation Evaluation Criteria**

<b>Criterion</b>	<b>Weight</b>
1. Clear research hypothesis & objectives	<b>10</b>
2. Concise description of approach and methods	<b>15</b>
3. Results and discussion: interpretation of results and critical analysis of their meaning and impact	<b>45</b>
4. Summary of findings and future plans	<b>10</b>
5. Ability of speaker to answer questions in a clear & meaningful manner.	<b>10</b>
6. Time management, visual media and speaker – audience contact	<b>10</b>

**MSc Final Project Presentation Evaluation Criteria**

<b>Criterion</b>	<b>Weight</b>
1. Concise, accurate & up-to-date literature review	<b>15</b>
2. Knowledge gap and/or problem clearly identified and stated	<b>15</b>
3. Clear research hypothesis & objectives; Concise description of approach and methods	<b>15</b>
4. Results and discussion: interpretation of results and critical analysis of their meaning and impact	<b>25</b>
5. Summary of findings and future plans	<b>5</b>
6. Time management, visual media and speaker – audience contact	<b>10</b>
7. Ability of speaker to answer questions in a clear & meaningful manner.	<b>15</b>



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## **PLAGIARISM**

Plagiarism is a serious offence. All students are expected to familiarize themselves with the Rhodes University Policy on Plagiarism:  
<https://www.ru.ac.za/media/rhodesuniversity/content/institutionalplanning/documents/Plagiarism.pdf>

Before lectures start, each student must sign the plagiarism declaration page and return to the course coordinator.

It is important to understand that in a senior course, a first offence is taken more seriously than in an introductory course.

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Student Name:

Student No:

**PLAGIARISM DECLARATION FORM**

1. I am aware of and I have familiarized myself with the Rhodes University Policy on Plagiarism:  
<https://www.ru.ac.za/media/rhodesuniversity/content/institutionalplanning/documents/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 theses, textbooks, journal articles AND on the internet.
3. I acknowledge and understand that plagiarism is wrong, and that it constitutes academic theft.
4. I understand that my research must be accurately referenced.
5. All the assignments that I submit during my MSc degree are my own work, or the unique work of a group, if a group assignment.
6. I have not allowed, nor will I in the future allow, anyone to copy my work with the intention of passing it off as his or her own work. I also accept that submitting identical work to someone else (a syndicate essay) constitutes a form of plagiarism.

Signed \_\_\_\_\_

Date \_\_\_\_\_

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**COURSE WORK MODULES**

***INTRODUCTION TO LINUX***

**Lecturer:** Prof Özlem Tastan Bishop and Dr Allan Sanyanga

**Contact hours:** 20

**SPECIFIC OUTCOMES ADDRESSED**

1. To be able to install a Linux operating system
2. Work comfortably and proficiently in Linux
3. To be able to install and use software in Linux
4. Master several shell commands

**BACKGROUND KNOWLEDGE REQUIRED**

Basic computer literacy: proficiency with word-processing, spreadsheets and graphics programs, exposure to standard bench-top computational tools and the web

**TEACHING METHODS/APPROACH**

The lectures will be complemented by tutorials and self-study

**BOOKS & OTHER SOURCES USED**

An Introduction to the Linux Command Shell for Beginners by Victor Gedris

GNU/Linux Command-Line Tools Summary by Gareth Anderson

Introduction to Linux – A Hand on Guide by Machtelt Garrels

**COURSE CONTENT**

1. Overview of Linux
2. Linux installation
3. Basic commands
4. The Linux file system
5. Working with files and folders in Linux
6. I/O redirection
7. Networking and connecting to an external server
8. Fundamental backup systems
9. Software management
10. Overview of Bash and Bash scripting
11. Miscellaneous advanced

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

1. Test 1: 40%
2. Test 2: 60%

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***PYTHON FOR BIOINFORMATICS***

**Lecturers:** Dr Allan Sanyanga

**Contact hours:** 80

**SPECIFIC OUTCOMES ADDRESSED**

1. To understand what programming is and why it is useful/necessary
2. To become familiar with the different variable types and data structures available in Python
3. To be able to write Python programs to solve basic problems
4. To be able to section off useful bits of code into Python functions
5. To understand and implement object-orientated programming
6. Advanced string handling
7. Reading and writing files
8. Useful modules and libraries (os, sys, numpy, scipy, pymol, args) and how to use them
9. Biological data analysis using Python
10. Handle errors efficiently and elegantly
11. Design and build command line tools with Python that adhere to best practices
12. Understand how to use an HPC cluster and submit jobs in a high throughput fashion

**BACKGROUND KNOWLEDGE REQUIRED**

Basic computer literacy; Basic understanding of the Linux operating system; Understanding of system directories

**TEACHING METHODS/APPROACH**

Teaching will consist of lectures and numerous small exercises and assignments to allow students to learn from practical experience

**BOOKS & OTHER SOURCES USED**

Python documentation: <http://docs.python.org/index.html>

Bioinformatics programming using python: Mitchell L model, O'Reilly

SAMs teach yourself python in 24 hours: Kate Cunningham

**COURSE CONTENT**

1. Introduction to Python
2. Numbers
3. Logic in Python
4. Strings, String formatting, user input and output
5. Data structures: Lists and Dictionaries
6. Repeating code with loops
7. Creating functions, Objects and Classes
8. Reading and writing files (text and spreadsheets)
9. Regular expressions

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**MSc PROGRAMME OUTLINE**

**MSc in Bioinformatics and Computational Molecular Biology**

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10. Useful modules in Python
11. Python interaction with the Linux bash subsystem (Advanced scripting) and cluster submission with python
12. Error handling
13. Tips and tricks

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

1. Daily exercises and assignments: 40%
2. Test: 20%
3. Project: 40%

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***BASIC GENOMICS***

**Lecturer:** Prof Özlem Tastan Bishop

**Contact hours:** 25

**SPECIFIC OUTCOMES ADDRESSED**

1. Become familiar with biological databases
2. Ability to retrieve and analyse data from biological databases
3. Understand various alignment algorithms
4. To be able to align homologous sequences in DNA or protein format and understand the advantages and disadvantages of the two approaches

**BACKGROUND KNOWLEDGE REQUIRED**

Basic biochemistry and genetics knowledge

**TEACHING METHODS/APPROACH**

The lectures will be complemented by tutorials, self-study and article discussions

**BOOKS & OTHER SOURCES USED**

1. Essential Bioinformatics by Jin Xiong
2. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
3. Manuals and tutorials of various sequence alignment programs
4. Research articles

**COURSE CONTENT**

1. Biological databases
2. Homology detection programs
3. Sequence alignment
  - a. Pairwise sequence alignment
  - b. Multiple sequence alignment
  - c. Profiles and HMMs
4. Sequence visualization programs

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

1. Small project: 50%
2. Test: 50%

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***STRUCTURAL BIOINFORMATICS – I***

**Lecturer:** Prof Özlem Tastan Bishop

**Contact hours:** 20

**SPECIFIC OUTCOMES ADDRESSED**

1. To understand structural biology terminology, especially X-ray crystallography
2. To learn how to use different protein visualization programs
3. To understand various secondary and tertiary structure prediction algorithms
4. To understand the range, applications and limitations of modeling methods
5. To learn and understand the various steps involved in homology modeling
6. To learn homology modeling using Modeller
7. To be able to use different model evaluation programs and understand how they work

**BACKGROUND KNOWLEDGE REQUIRED**

1. Knowledge on biochemical properties of amino acids
2. Basic understanding of primary, secondary, tertiary and quaternary protein structure
3. Knowledge on non-covalent bond formations

**TEACHING METHODS/APPROACH**

The lectures will be complemented by tutorials, self-study and article discussions

**BOOKS & OTHER SOURCES USED**

1. Essential Bioinformatics by Jin Xiong
2. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
3. Molecular Modeling and Simulation - An Interdisciplinary Guide by Tamar Schlick
4. Manuals and tutorials of various modeling and visualization programs

**COURSE CONTENT**

1. Structural biology techniques
2. The Protein Data Bank
3. Protein visualization programs
4. Protein secondary and tertiary structure prediction
5. Homology modeling with Modeller
6. Model validation programs

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

1. Small project:           50%
2. Test:                     50%

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***STRUCTURAL BIOINFORMATICS – II***

**Lecturer:** Dr. Kevin A. Lobb

**Contact hours:** 25

**SPECIFIC OUTCOMES ADDRESSED**

This course introduces the theory and practice of molecular modelling as used in chemistry and medicinal chemistry. Although competence in the use of several software packages is a critical component, emphasis will be on the understanding of the methods and on strategies in their application to a wide variety of problems.

**BACKGROUND KNOWLEDGE REQUIRED**

Little background knowledge is required, beyond that of basic chemistry. However it is essential that you are comfortable with chemical structures and that you can quickly identify whether they are correct or incorrect in terms of positioning and the valency of atoms. Familiarity with the any following concepts would be helpful, though not essential as we will deal with what is necessary during the course. Conformational analysis (e.g. boat and chair cyclohexane); orbitals, HOMO, LUMO, bonding and antibonding, excited state; Infrared Spectroscopy; transition state; activation energy; enthalpy, entropy and free energy.

**TEACHING METHODS/APPROACH**

The teaching will be split equally between lectures and practicals.

**BOOKS & OTHER SOURCES USED**

User manuals and background from the programmes Maestro, Gaussian, GAMESS, Autodock, Vega ZZ, KNIME and relevant supplied journal articles.

**COURSE CONTENT**

Theories used in calculations, molecular mechanics, semi-empirical, Hartree-Fock, configuration interaction and density functional theory. Correlation energy. Basis sets. Strategies for dealing with extremely large systems. Combined methods QM/MM, ONIOM, discrete and continuum solvation. Exploring the potential energy surface and vibrational analysis. Conformational searches. Calculable properties. Excited states. Calculations in vacuo, periodic boundary conditions.

Chemical Libraries. Molecular docking – construction of small molecules, preparation of protein and the docking procedure. Docking via scripting, and high-throughput virtual screening.

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

There will be an assignment which will make up 100% of the mark for this course.



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***STRUCTURAL BIOINFORMATICS – III***

**Lecturer:** Dr Vuyani Moses

**Contact hours:** 25

**SPECIFIC OUTCOMES ADDRESSED**

This course will introduce the principle of Molecular Dynamics (MD) simulations to study protein-ligand interactions. This will require the docked protein-ligand complex that would have been generated in the “STRUCTURAL BIOINFORMATICS II” course.

**BACKGROUND KNOWLEDGE REQUIRED**

This course will require basic understanding of protein systems, in particular protein-ligand complexes and metal containing enzymes interactions.

**TEACHING METHODS/APPROACH**

This course will be a combination lectures and practicals/tutorials

**BOOKS & OTHER SOURCES USED**

Reading the user manuals and the tutorials of the programs to be used will be advantageous.

The programs to be used are:

CHARMM

GROMACS

Gaussian09

**COURSE CONTENT**

1. The principles of Molecular dynamics simulations of protein-ligand complexes (in GROMACS).
  - i. Structure preparation
  - ii. Solvation
  - iii. Neutralization
  - iv. energy minimization
  - v. Equilibration
2. Trajectory analysis:
  - i. Root Mean Square Deviation
  - ii. Radius of gyration
  - iii. Potential energy
  - iv. Visualization in VMD

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

Assignment    50%

Test            50%

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***STRUCTURAL BIOINFORMATICS – IV***

**Lecturer:** Dr Vuyani Moses

**Contact hours:** 25

**SPECIFIC OUTCOMES ADDRESSED**

In cases where there are no force field parameters for part of the system to be simulated, force field parameters may be generated by Quantum Mechanics and Molecular Mechanics (QM/MM) studies. As a result, the aim of this course will focus on generating force field parameters for metal containing systems.

**BACKGROUND KNOWLEDGE REQUIRED**

This course requires successful completion of the Structural Bioinformatics III course and an understanding of protein structure and function.

Reading the user manuals and the tutorials for the Gaussian09 program will also be advantageous.

**TEACHING METHODS/APPROACH.**

This course will be taught by lectures followed by hands on practical sessions.

**BOOKS & OTHER SOURCES USED**

Research articles pertaining to the methodologies of interest will be presented in class.

**COURSE CONTENT**

Force field parameter generation:

1. Subset creation (QM) vs ONIOM calculations(QM/MM)
2. QM/MM potential energy surface scans (PES) (in Gaussian09)
3. Force field selection
4. List squares fitting to generate force field parameters
5. Atom names vs Atom types
6. MD simulations to validate force field parameters (in CHARMM)

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

Test	50%
Assignment	50%

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***INTRODUCTORY STATISTICS***

**Lecturer:** Mr. Jeremy Baxter

**Contact hours:** 25

**SPECIFIC OUTCOMES ADDRESSED**

The aims of this course are:

1. To provide students with the basics of probability theory (probability, probability axioms, conditional probability, probability density function, cumulative distribution function, expectation, variance, discrete random variable, continuous random variable) and statistical background, concepts and techniques (statistical experiment, descriptive statistics, inference statistics) that are most useful to Bioinformaticians.

On completion of the course students should, inter alia, be able to:

1. Explain the differences between a population and a sample.
2. Collect, summarise and describe data using suitable numerical and graphical techniques.
3. Explain the concepts of probability, interpret probabilities and use suitable theory to calculate simple and conditional probabilities.
4. Identify discrete and continuous probability distributions.
5. Demonstrate the use of the binomial, Poisson, normal, Student t, chi-square and F distributions.
6. Calculate point and interval estimates, one- and two-sample, for the population mean(s), proportion(s) and variance(s) and interpret the meaning of each.
7. Perform suitable hypothesis tests (parametric and or non-parametric procedure) for one- and two-sample analyses and draw meaningful conclusions and decisions for the population mean(s), proportion(s) and variance(s).
8. Estimate, interpret and make predictions using linear models. Perform suitable statistical inference and model diagnostics for linear models.

**BACKGROUND KNOWLEDGE REQUIRED**

1. Basic Calculus: Differentiation and integration
2. Linear algebra: Matrices, vectors
3. Matlab literacy, specifically matrix operations.
4. Basic programming experience, in python or perl

**TEACHING METHODS/APPROACH**

This course will be taught using formal lectures, typically in the morning, and self-study tutorials and practicals. Use of hand-outs, notes, text books, board-work and overheads. Relevant notions from linear algebra and statistics will be discussed and the student will then be required to read portions of prescribed texts on his/her own. At each lecture a set of exercises will be presented and completed ready for assessment by the next lecture.

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**BOOKS & OTHER SOURCES USED**

1. J Baxter, Introductory Statistics for Bioinformaticians using R (course notes/slides).
2. Wim P. Krijnen, 2009, Applied Statistics for Bioinformatics using R, CRAN

**COURSE CONTENT**

1. A brief introduction to R.
2. Descriptive statistics (Graphical and numerical summaries of univariate, bivariate and multivariate data).
3. An introduction to statistical distributions.
4. Estimation and inference for one/ two random samples (Parametric and non parametric methods.)
5. An introduction to correlation, linear regression and linear models: (One and Two Way ANOVA)

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

1. Daily assignments/exercises: 40%
2. Tests: 60%

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***MATLAB AND ARTIFICIAL NEURAL NETWORKS***

**Lecturer:** Prof Nigel Bishop

**Contact hours:** 25

**SPECIFIC OUTCOMES ADDRESSED**

Describe biological/bioinformatics problems using mathematics. Solve these problems using calculus, linear algebra. Introduce students to the mathematical programming environment MATLAB, and use it to solve problems. Use of artificial neural networks in MATLAB.

**BACKGROUND KNOWLEDGE REQUIRED**

Basic calculus and linear algebra.

**TEACHING METHODS/APPROACH**

This course will be a combination of lectures and practicals /tutorials

**BOOKS & OTHER SOURCES USED**

User Manuals for MATLAB and mathematics textbooks.

**COURSE CONTENT**

Calculus (differentiation and integration); linear algebra (matrices, eigenvalue / eigenvector problems).

Introduction to the MATLAB environment; programming in MATLAB: statements, data structures, input / output, flow control, functions, plotting of graphs in 2D and 3D.

Linear algebra with MATLAB: systems of equations, over-determined systems and linear regression, eigenvalues and eigenvectors. Other applications: differentiation, integration, solving nonlinear equations and differential equations.

Artificial neural networks (ANN) with MATLAB: construct, train and use ANN to solve scientific problems.

**ASSESSMENT ACTIVITIES AND THEIR WEIGHTS**

Daily assignments      50%

Test                              50%

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**CONTACT DETAILS OF LECTURERS & SUPERVISORS**

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