QUALITY ASSURANCE MANUAL
DEPARTMENT OF BIOCHEMISTRY, MICROBIOLOGY AND BIOTECHNOLOGY

MSc PROGRAMME OUTLINE **MSc in Bioinformatics and Computational Molecular Biology**		
Course Work / Project Masters	**Year: 2014**	**Coordinator: Prof Özlem TAŞTAN BISHOP**

COURSE WORK and RESEARCH PROJECT MASTERS

in

BIOINFORMATICS and
COMPUTATIONAL MOLECULAR BIOLOGY

2014

DEPARTMENTS

of

BIOCHEMISTRY & MICROBIOLOGY

CHEMISTRY, COMPUTER SCIENCE, MATHEMATICS and STATISTICS

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ORIENTATION DAY

(13 February 2014, Thursday)

(Place: RUBi Lab 129A, Biological Sciences Building 1st Floor)

8:30 – 9:00 Welcoming and tea/coffee/scone

9:00 – 10:15 Introduction of students, lecturers, supervisors, rest of RUBi members

(Place: Biochemistry Seminar Room 1, Biological Sciences Building 5th Floor)

10:30 – 11:00 "Introduction to the programme" by Prof Özlem Taştan Bishop

11:00 – 11:30 "What is plagiarism? – Part 1" by Prof Philip Machanick

11:30 – 13:00 Research talks with some examples from previous MSc projects (20 min each, 10 min for questions)

- 11:30 - Dr Kevin Lobb
- 12:00 - Prof Philip Machanick
- 12:30 - Prof Özlem Taştan Bishop

14:00 – 15:00 Laptops will be given to the students who completed the registration process (RUBi Lab 129A)

15:00 – 15:30 "What is plagiarism? – Part 2" by Prof Philip Machanick

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PROPOSED PROGRAMME FOR 2014

Date	Module	Content
13 **Feb**, Thu	**ORIENTATION DAY**	
14 **Feb**, Fri	**Research project discussion with supervisors** *(Time will be arranged by supervisors)*	
17 -21 **Feb** 3-14 **Mar** 31 **Mar** – 4 **Apr** [20 contact hours]	**Biochemistry 2 (Building blocks) BCH201** BP, HH and AE	• Building blocks (BP) • Amino acids (HH) • DNA/RNA (AE) (For students who have no biology background)
17 **Feb**, Mon - 21 **Feb**, Fri [20 contact hours]	**Introduction to Linux** Prof Özlem Taştan Bishop Tutor – N. Faya	• Linux operating system and software installation • Use of Linux and Linux shell commands • Application to Bioinformatics problems
24**Feb,** Mon **–** 28 **Feb,** Fri [10 hours]	**Introduction to Programming** Prof Philip Machanick Tutor – Caleb Kipkurui	Basics for (Python) programming
3 **Mar,** Mon **–** 5 **Mar,** Wed [15 hours]	**Introduction to Mathematics** Prof Mike Burton	Review of basic calculus and linear algebra

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6 **Mar,** Thur **–** 11 **Mar,** Tue [20 hours]	**Mathematical Programming** Prof Mike Burton Prof Nigel Bishop	The MATLAB computational environment, MATLAB scripts, graphical output, functions, systems of linear and non-linear equations, differential equations. Use of the Bioinformatics Toolbox.
12 **Mar,** Wed**,** 13 **Mar,** Thu, 21 **Mar**, Fri	**Study days**	
14 **Mar**, Fri 17 **Mar,** Mon **–** 20 **Mar,** Thu [25 hours]	**Basic and Advanced Genomics – Part 1** Prof Özlem Taştan Bishop Mr David Brown Tutors – Candice Ryan & Vuyani Moses	DNA and protein databases; database searching; sequence alignment Databases and API
24 **Mar**, Mon – 28 **Mar**, Fri [25 hours]	**Basic and Advanced Genomics – Part 2** Prof Philip Machanick Tutor - Caleb Kipkurui	Discovering features of interest in DNA including transcription factor binding sites, using genome browsers to obtain data, using web services and the command line to performance genome-wide and specific sequence analyses
31 **Mar**, Mon – 17 **Apr**, Thu [75 hours]	**Python for Bioinformatics** Mr Gustavo Adolfo Salazar Orejuela Tutors - Caleb Kipkurui & N. Faya	• Introductory and advanced Python • Biopython
18 **Apr**, Fri – 21 **Apr**, Mon	**Easter holiday**	
22 **Apr**, Tue – 28 **Apr**, Mon	**Python (assignment week)**	

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29-30 **Apr** , 2 **May**	**Study days**	
5 **May**, Mon – 9 **May**, Fri	**EXAMINATIONS:** • **Linux** (5 May) • **Basic mathematics and Matlab** (6 May) • **Basic genomics I** (7 May) • **Basic genomics II** (8 May) • **Python** (9 May)	
12 **May**, Mon - 16 **May**, Fri [25 hours]	**Structural Bioinformatics I** Prof Özlem Taştan Bishop Tutors – Thommas Musyoka & Vuyani Moses	Protein visualization programs; structural biology techniques; template and non-template based protein structure prediction methods; homology modeling
19 **May**, Mon - 23 **May**, Fri [25 hours]	**Structural Bioinformatics II** Dr Kevin Lobb Tutor – Thommas Musyoka & Candice Ryan	Molecular dynamics; protein-small molecule interactions; Autodock.
26 **May**, Mon - 30 **May**, Fri [25 hours]	**Comparative genomics** Prof Oleg Reva	Introduction to pairwise and multiple complete genome alignment; phylogenomics; genome evolution; and horizontal gene transfer. New approaches, techniques and challenges.
2 **June,** Mon– 6 **June,** Fri [25 hours]	**Statistics** Mr Jeremy Baxter	Introductory statistics; R: statistical software

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9 June, Mon - 13 June, Fri **[25 hours]**	**Databases** Mr Rowan Hatherley Mr David Brown	• Introduction to databases • Introduction to web frameworks • MySQL; Django
16 **June**, Mon – 20 **June**, Fri	**Study week**	
23 **Jun**, Mon – 27 **Jun**, Fri	**EXAMINATIONS:** • **Structural Bioinformatics I** (23 June) • **Structural Bioinformatics II** (24 June) • **Comparative genomics** (25 June) • **Statistics** (26 June) • **Databases** (27 June)	
30 **Jun,** Mon – 6 **Jul,** Sun	**BREAK**	
15 **Jul,** Tue	**PROJECTS:** Hand-in Literature Review and Project Proposal to Supervisor and Co-supervisor – **Project starts!**	
21 **Jul,** Mon	**PROJECTS:** Project Proposal Presentations	
6 **Aug**, Wed – 19 **Nov**, Wed	**BIOINFORMATICS JOURNAL CLUB**	
Week of 22 **Sep**	1st Presentation of Project Progress	
Week of 20 **Oct**	2nd Presentation of Project Progress	
Week of 24 **Nov**	Presentation of project results	
10-14 **Dec**	**Thesis submission (If thesis on time)**	

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OVERALL TEACHING HOURS

	Contact Hours	Lecturing Hours	Practicals and tutorials
(Basic Biochemistry)	(20)	(20)	0
Introduction to Linux	20	9	11
Introduction to Mathematics	15	7	8
Mathematical programming	20	9	11
Basic & Advanced Genomics I	25	11	14
Basic & Advanced Genomics II	25	11	14
Python for Bioinformatics	75	34	41
Structural Bioinformatics I	25	11	14
Structural Bioinformatics II	25	11	14
Comparative genomics	25	11	14
Statistics	25	11	14
Databases	25	11	14
TOTAL	305	136	169

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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

Module	**Weighting**	**Duration (hours)**
Introduction to Linux	6.6 %	2
Mathematics	4.9%	2
Mathematical programming	6.6%	2
Basic and Advanced Genomics I	8.2%	3
Basic and Advanced Genomics II	8.2%	3
Python for Bioinformatics	24.6%	4-5
or		
(Python for com. sci students)	*18.0%*	*4-5*
Introductory biochemistry	*6.6%*	*will be defined later*
for non-biology background students)		
Structural Bioinformatics I	8.2%	3
Structural Bioinformatics II	8.2%	3
Comparative genomics	8.2%	3
Statistics	8.2%	3
Databases	8.2%	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.

- **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.

5. 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.

6. 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

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

MSc Written Proposal Evaluation Form

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

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MSc Project Progress Presentation Evaluation Criteria

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

MSc Final Project Presentation Evaluation Criteria

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

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PLAGIARISM

Plagiarism is a serious offence. All students are expected to familiarize themselves with the Rhodes University Policy on Plagiarism:
http://www.ru.ac.za/static/policies/plagiarism_policy.pdf

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

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Student Name:

Student No:

PLAGIARISM DECLARATION FORM

1. I am aware of Rhodes University Policy on Plagiarism webpage and I have familiarized myself (http://www.ru.ac.za/static/policies/plagiarism_policy.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 Taştan Bishop
Contact hours: 20

SPECIFIC OUTCOMES ADDRESSED

1. To be able to install a Linux operating system
2. To be able to install various programs
3. Log in and out of a Linux system
4. Work with directories and files and change file permissions
5. Master several shell commands
6. Redirect input and output and print documents

BACKGROUND KNOWLEDGE REQUIRED
Basic computer literacy: proficiency with word-processing, spreadsheets and graphics programmes, 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
Introduction to Linux – A Hand on Guide by Machtelt Garrels (tldp.org/LDP/intro-linux/intro-linux.pdf)

COURSE CONTENT

1. What is Linux?
2. How to install an operating system
3. Quick start
4. About files and file systems
5. Processes
6. I/O redirection
7. Text editors
8. Home
9. Printers and printing
10. Fundamental backup systems
11. Networking
12. Installation of various programs

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

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

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INTRODUCTION TO PROGRAMMING
Lecturer: Prof Philip Machanick
Contact hours: 10

This is an introductory module to prepare students for programming. Students will not be examined on this module.

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BASIC MATHEMATICS
Lecturer: Prof Mike Burton
Contact hours: 15

SPECIFIC OUTCOMES ADDRESSED
1. Describe biological/bioinformatics problems using mathematics.
2. Solve these problems using calculus, linear algebra.
3. Acquire background for Matlab and Statistics courses

BACKGROUND KNOWLEDGE REQUIRED
Basic calculus, algebra, linear algebra

TEACHING METHODS/APPROACH
The lectures will be complemented by self-study and tutorials.

BOOKS & OTHER SOURCES USED
Lecture notes
Any Calculus, Linear Algebra books

COURSE CONTENT
1. Calculus (Differentiation and integration)
2. Linear Algebra (Matrices, eigenvalue / eigenvector problems)

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS
1. Assignment 1: 25%
2. Assignment 2: 25%
3. Test: 50%

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MATHEMATICAL PROGRAMMING WITH MATLAB
Lecturer: Prof Mike Burton and Prof Nigel T. Bishop
Contact hours: 20

SPECIFIC OUTCOMES ADDRESSED
1. Introduction to mathematical programming with MATLAB.
2. Solve problems using mathematical programming.

BACKGROUND KNOWLEDGE REQUIRED
Matrix algebra, basic calculus.

TEACHING METHODS/APPROACH
Lectures will be mainly in the form of demonstrations of MATLAB features, with discussion. Relevant notions from various aspects of mathematics will be discussed as necessary. At each lecture a set of exercises will be presented, which students should complete and submit by the next lecture.

BOOKS & OTHER SOURCES USED
Course notes.
Essential MATLAB for Scientists and Engineers, B Hahn, Pearson, 3 rd edition ISBN 1 868 91143 82

COURSE CONTENT
The purpose of the course is to enable the student to construct a computational environment with MATLAB in which to model, study and simulate real-world processes. It is intended that the student learn this skill by hands-on experience with the computer. The lectures are meant to provide an overview and a forum for discussion. The exercises are there to provide practical experience. Most of the real learning will be accomplished by doing the exercises.
1. Introduction to the MATLAB environment; programming in MATLAB: statements, data structures, input / output, flow control, functions, graphics
2. Linear algebra with MATLAB and maxima: systems of equations, over-determined systems and linear regression, eigenvalues and eigenvectors
3. Other applications of MATLAB: differentiation, integration, solving nonlinear equations and differential equations.

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS
1. Assignment 1: 20%
2. Assignment 2: 20%
3. Project: 60%

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BASIC GENOMICS - I
Lecturer: Prof Özlem Taştan Bishop
Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

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

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. Introduction to bioinformatics by Anna Tramontano
3. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
4. Research articles and other bioinformatics books in the library

COURSE CONTENT

1. Biological databases
2. Databases and API
3. Sequence alignment
    a. Pairwise sequence alignment
    b. Database similarity search
    c. Multiple sequence alignment
    d. Profiles and HMMs

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 25%
2. Assignment 2: 25%
3. Test: 50%

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BASIC GENOMICS - II
Lecturer: Prof Philip Machanick
Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED
Understanding how DNA is computationally analysed for features of interest, including but not limited to transcription factor binding sites.

BACKGROUND KNOWLEDGE REQUIRED
Role of DNA in genetics, basic understanding of developmental biology.

TEACHING METHODS/APPROACH
Lecturing, demonstrating techniques and problem-solving.

BOOKS & OTHER SOURCES USED
Web searches and academic literature.

COURSE CONTENT

1. Transcription factors and how they relate to DNA
2. How transcription facror binding is modeled using motifs
3. Sources of known motifs
4. Determining binding specificity including comparative methods
5. Web-based and scripting approaches

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 40%
2. Assignment 2: 60%

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PYTHON AND BIOPYTHON
Lecturer: Mr Gustavo Salazar
Contact hours: 75

SPECIFIC OUTCOMES ADDRESSED

1. To be able to write short Python program to manipulate data
2. To understand the differences between numbers, strings, lists and arrays
3. To master the use of various control structres and functions within Python program
4. To understand the concepts of the Object Oriented paradigm and how to use it in python
5. To retrieve and manipulate data from databases and files
6. To use the most common procedures in Biopython

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

TEACHING METHODS/APPROACH
Lectures: utilizing self-study tutorials and demonstration programmes
Numerous small exercises to build up experience and skills progressively

BOOKS & OTHER SOURCES USED
Python documentation: http://docs.python.org/index.html
Biopython http://biopython.org/wiki/Biopython

COURSE CONTENT

1. Introduction to Python (Thinking, writing and running)
2. Flow Control
3. Data Structures
4. Strings in Depth
5. Functions
6. Importing Standard Modules
7. Files for Input and Output
8. Regular Expressions
9. Basic Parsing
10. Exceptions and error handling
11. Recursion
12. Classes and Objects
13. Database Theory and Relational Databases
14. Biopython
15. Graphical User Interfaces

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ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Test: 30%
2. Mini-project: 30%

Assignments: 40%

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STRUCTURAL BIOINFORMATICS – I
Lecturer: Prof Özlem Taştan Bishop
Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To understand structural biology terminology, especially X-ray crystallography, and to be able to follow the literature
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 modeling by using Modeller

BACKGROUND KNOWLEDGE REQUIRED

1. Knowledge on biochemical properties of amino acids
2. Basic understanding of the primary, secondary, tertiary and quaternary structure of proteins.
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. Introduction to bioinformatics by Anna Tramontano
3. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
4. Manuals and tutorials of various modeling and visualization programs

COURSE CONTENT

1. Structural biology techniques
2. Protein visualization programs
3. Protein secondary structure prediction
4. Protein tertiary structure prediction
5. Homology modeling; Modeller

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment: 20%
2. Short project: 40%
3. Test: 40%

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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 programs Materials studio, Gaussian, CHARMM, GAMESS, VASP, Autodock, Vega ZZ, CPMD, Sparky 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. Molecular dynamics (MM, Born-Oppenheimer and Car-Parrinello). Interaction between systems – basis set superposition error, protein-small molecule interactions and docking. NMR – relaxation, coupling and relevant experiments used in biomolecular NMR. Principles of structure assignment. Protein-ligand interactions by NMR.

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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COMPARATIVE GENOMICS
Lecturer: Prof Oleg Reva
Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To understand opportunities, challenges and possible pitfalls of comparison of complete genomes;
2. To get known available resources (databases and open source programs);
3. To learn how to use different genome comparison programs;
4. To understand the concepts of genomic polymorphism; gene homology; genomic evolution and horizontal gene transfer;
5. To gain practical skills in using genome comparison programs and techniques.

BACKGROUND KNOWLEDGE REQUIRED

1. Basic knowledge of genetics of eukaryotes and prokaryotes.
2. Basic computer skills on Windows PC.

TEACHING METHODS/APPROACH
The lectures will be complemented by tutorials.

BOOKS & OTHER SOURCES USED

1. Analysis of genes and genomes by Richard J. Reece;
2. Bioinformatics – a practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette;
3. Systems and computational biology – molecular and cellular experimental systems by Ning-Sun Yang;
4. Manuals and tutorials of various modeling and visualization programs.

COURSE CONTENT

1. Introduction to genome alignment approaches;
2. Introduction to the concepts of genome polymorphism;
3. Introduction to genome evolution and horizontal gene transfer;
4. Introduction to phylogenomics;
5. Selection and use of various software tools for comparative genomics: practical course.

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

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

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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

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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.

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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DATABASES
Lecturers: Mr Rowan Hatherley & Mr David Brown
Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To understand what databases are and why they are used
2. To be able to create and manage a simple database using MySQL
3. To understand what a web framework is and why it is used
4. To create simple web pages using Django
5. To create and manage a simple online database using Django and MySQL

BACKGROUND KNOWLEDGE REQUIRED

1. Basic computer literacy
2. Basic Python programming skills

TEACHING METHODS/APPROACH

Teaching will consist of lectures, practicals and tutorials.

BOOKS & OTHER SOURCES USED

Course notes and lecture slides, The Django website (www.djangoproject.com), the MySQL website (www.mysql.com), http://www.w3schools.com, other web searches and online tutorials

COURSE CONTENT

1. Introduction to databases and DBMs
2. Database design
3. SQL and MySQL
4. Introduction to web frameworks
5. Django

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Daily practicals and tutorials 60%
2. Test 20%
3. Assignment 20%

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