BIOINFORMATICS, UNDERGRADUATE STUDY PROGRAMME, FIRST BOLOGNA CYCLE

COURSE DESCRIPTIONS

COMPULSORY COURSES

COMPULSORY COURSES OF THE 1ST YEAR OF STUDY

Course name: **ANALYSIS I - FOUNDATIONS OF ANALYSIS**
Number of ECTS credits: **6**

Content:
- The natural numbers. Rational numbers. Real numbers. Complex numbers.
- The sequence of real numbers. Limits and accumulation points. Cauchy condition. Upper and lower limit. Monotone sequences. Bolzano-Weierstrass theorem.
- Series. The convergence criteria. Absolutely and conditionally convergent series.
- Functions of real variables, even and odd functions, periodicity. Limits of functions, left and right limits. Continuity. Continuous functions on closed intervals limited. Bisection method for finding zeros.
- The elementary functions. Cyclometric functions.

Course name: **ALGEBRA I - MATRIX CALCULUS**
Number of ECTS credits: **6**

Content:
- Vectors, analytic geometry in space.
- Matrices. Types of matrices and basic operations with matrices. Rank of a matrix. Inverse. Systems of linear equations. Matrix interpretation and theorem of solvability. Elementary matrices, Gauss method. Determinants. Cramer's rule.

Course name: **ANALYSIS II – INFINITESIMAL CALCULUS**
Number of ECTS credits: **6**

Content:
- Derivative. Mean value theorems. Differentiation of monotone functions. L'Hopital's rule. Higher derivatives. Taylor's formula. Local extrema. Convex and concave functions. Inflection points. Tangent method of finding the zeros.
- The indefinite integral. Definite Integrals. Darboux and Riemann sums. Leibniz-Newton formula. Mean value theorems. Integration methods. Applications of the definite integral in geometry. Improper integral. Numerical integration.
- The logarithm, the number e, and the definition of exponentiation with the real exponent.
- Drawing planar curves.
- Sequences and function series. Power series. Taylor series. Elementary
- complex functions.

Course name: **PROGRAMMING I**
Number of ECTS credits: **6**

Content:
The course will cover topics that might include (but are not restricted to) any of the following according to the needs and development of the subjects covered:

- Basic building blocks of a computer program.
- Basic syntax of the programming language Java:
- Variables, types and expressions. Basic I/O operations. Decision statements. Control structures. Functions and parameters. Programs. Structural decomposition.
- Basic data structures:
- Simple types. Arrays. Records. Characters and strings. Data representation in computer memory. Memory allocation. Linked structures. Stack. Queue. List. Tree.
- Algorithms and problem solving:
- What is an algorithm? Problem solving strategies. The role of algorithms in problem solving. Algorithm implementation strategies. Debugging. Recursion – recursive functions, divide-and-conquer principle, backtracking, implementation of recursion.
- Programming languages overview:
- Types of programming languages. Flow control. Functions. Subprograms. Namespaces.
- Declarations and types:
- Types. Declarations of types. Safe typing. Type checking. Subtypes. Classes. Polymorphism.
- Abstraction mechanisms:
- Data abstractions. Simple types. Composite types. Flow abstractions. Subprograms and functions. Abstract data types. Objects and classes. Patterns. Modules.

Course name: **COMPUTER PRACTICUM**
Number of ECTS credits: **6**

Content:
The course will cover topics that might include (but are not restricted to) any of the following according to the needs and development of the subjects covered:

The faculty network and basic usage rules:
- Description of the faculty computer network, login methods, password changing procedure, e-mail and mailing list usage, access to e-materials.

OS Linux basics:
- Description of the Linux OS and its many flavors, BASH shell usage basics.

Programming language C:
- The syntax of the C programming language and its usage to solve simple problems.

Course name: **GENERAL AND INORGANIC CHEMISTRY**
Number of ECTS credits: **6**

Content:
The course presents the basic chemical laws. Students learn the basics of quantitative characteristics and structure of matter, chemical processes and electronic configuration of atom, types of chemical bonds, chemical reactions, chemical equilibrium and energy changes in chemical reactions.
The first part is made from brief summary of the substance and material changes and chemical laws; second part is upgraded with explanation of basic chemical concepts: atom, molecule, ion, element, compound, substance, mixture, formulas, etc. Students are introduced to the computational exercises. Scope of atomic and chemical bonds is focused on the importance of the chemical bonds within atoms and molecules and on the structure of periodic table of elements. A basic overview of the dispersants systems and chemical equilibrium within the reactions. Review of inorganic compounds is given according to the periodic table of elements and review of organic compounds is with functional groups. Students acquire the basic chemical education which is key to every naturalist, and his effect on the

labor market. At the same time, students learn to use critical analysis and development, practical application of theories in solving practical problems in the field of chemistry. The subject is the basis for other chemical objects in the program, and serves as a balancing of chemical knowledge, which the students bring from high school. Students upgrade theoretical knowledge acquired by lectures, with practical examples in the context of computational and laboratory exercises.

Course name: **PROGRAMMING II – CONCEPTS OF PROGRAMMING LANGUAGES**
Number of ECTS credits: **6**

Content:
The course will cover topics that might include (but are not restricted to) any of the following according to the needs and development of the subjects covered:
- Introduction
- Lambda calculus
- Syntax
- Basic structures
- Functional languages
- Imperative languages
- Types
- Modules
- Objects and classes

Course name: **INTRODUCTION TO GENETICS AND GENOMICS**
Number of ECTS credits: **6**

Content:
Course name: **INTRODUCTION TO GENETICS AND GENOMICS**
Number of ECTS credits: **6**

Content:
- Fundamentals of transmission genetics: lows of inheritance, pedigree analysis of inheritance of dominant and recessive genes, molecular basics of dominant and recessive mutations.
- Avtosomal and sex linked inheritance.
- Cytoplasmic inheritance.
- Human genome organization.
- Genome mapping, techniques of mapping, genetic and physical approaches, PCR technique, Southern, Northern detection, DNA markers (RFLP, VNTR, SSR, SNP, EST, AFLP…), fluorescent in situ hybridization (FISH), mapping STS
- Restriction enzymes, separation of DNA fragments, cloning DNA vectors
- DNA recombinant techniques
- Methods for sequencing DNA, understanding and importance of genomic projects
- Analysis of genes, reverse genetics, methods for analysis of expressed sequences
- Morphology and structure elements of Eukaryote chromosome: telomere, centromere, role, replication model of telomere, organization of DNA on the chromosome, construction of chromatin, heterochromatin
- Organization of Eukaryote genome
- Genes and organization of genes
- Organel genomes, evolution and properties
- The path from DNA to protein
- Expression of genes: initiation of transcription, the role of chromatin, the role of RNA polymerases, regulation of transcription in prokaryotes and eukaryotes, positive and negative regulation of expression of genes.
- Synthesis and processing of different RNA molecules
- Modification of genetic material, mutations on the chromosome, gene, genome. The causes of mutations, the impact on the organism and the importance in the evolution
- Repair mechanisms

- Recombinations
- Mobile genetic elements and their role
- Evolution of genomes
- Population genetics: genetic variability and changes in populations, genetic distances, methods for estimation of genetic variability and distances, molecular markers for population genetic studies
- Application of genomics

Course name: **GENERAL BOTANY**
Number of ECTS credits: **6**

Content:
During the course, the students will become acquainted with the basic structure of the plant organism at the level of macromolecules, subcellular microstructures, cells, tissues and the whole organism. Emphasis will also be placed on the adaptations of plants living in different environments both at the cellular, anatomical and morphological level. Students will gain knowledge about the basic principles and forms of reproduction. The course will focus on delivering the basic knowledge needed to understand the contents of other related subjects. The course is adapted to a relatively wide range of students of other study programmes in the field of science.

Main issues:
- Morphology and anatomy of plants
- Cytology - the science of cell
- Histology - the science of tissues
- Stem
- Leaves
- Roots
- Secondary growth of plants
- Flowers and Reproduction

Course name: **GENERAL ZOOLOGY**
Number of ECTS credits: **6**

Content:
The course is an introduction to zoology, which gives a fundamental understanding of the structure and function of animals. Students are introduced to the principles of biology and theoretical basis for defining species, to the basic of Darwin-Wallace theory of evolution, and to the theory on the origin of life. They learn about the structure of animals through the basic levels of organization of living matter, i.e. through cytology, histology, morphology and organography. The function of each system is given by the integral structure.

The focus of the course is on the phylogenetic classification of animals presented through the main taxonomic groups (phyla). Students are first introduced to the history of classification, principles of zoological nomenclature and basics of animal systematic presented in an evolutionary context with emphasis on the understanding of animal body plans (body symmetry), development of germ layers, body cavities and embryonic development- Through this course student will be trained in critical assessment of various systems, which are perceived as hypothesis rather than a fact. The course also includes visiting lecture of an invited expert in certain field of zoology, and discussion/ synthesis of the knowledge obtained through this course.

Main Themes:
- principles of biology, functional and structural characteristics of organisms;
- origin of life; organic evolution, evolution of cell and multicellular organisms;
- Darwin – Wallace theory of evolution; mikroevoltion and macroevolution;
- theory of species; classification and systematic of animals;
- cytology, histology, organography and morphology of animals;
- reproduction and ontogeny of animals;

- introduction animal ecology and ethology.

COMPULSORY COURSES OF THE 2ND YEAR OF STUDY

Course name: **BASIC PHYSICS WITH BIOPHYSICS**
Number of ECTS credits: **6**

Content:
The subject presents a comprehensive basis of physics and biophysics both in its theoretical and practical aspects. We introduce the basic physical concepts, which are the basis for understanding processes in living beings. The importance of these concepts is further fortified with explanations and with real examples. Students learn about the rich and additive physical quantities and operating procedures for measuring these quantities, forms of energy, material, electrical and thermal currents, conservation laws, oscillations and waves. They accurately understand biophysical applications such as biomechanics, pressure and concentration differences as a cause for material flows, temperature differences as a cause for heat flow, potential difference as the cause for electrical currents, vocal chords as sound transmitter and biophysical structure of ears as a sound receiver, optical instruments and basics of molecular biophysics. Physics and biophysics are an essential part of the study and understanding of physical phenomena in chemistry, biology and medicine, as in ecology. Students are acquainted with the understanding of theoretical and practical problems that they will encounter in laboratory research work, or in industry.

Course name: **THEORETICAL COMPUTER SCIENCE I**
Number of ECTS credits: **6**

Content:
The course will cover topics that might include (but are not restricted to) any of the following according to the needs and development of the subjects covered:

- Fundamentals of mathematical theory, propositional calculus, truth tables, predicate calculus.
- Formal languages.
- Basic concepts of mathematical logic.
- Ways of describing sets. Basic relations between sets, basic operations on sets or families of sets. Power set. Relations. Graphs. Equivalence relations. Partial and linear ordering. Lattices and Boolean algebra. Well-ordered sets. Functions. Special types of functions. Categories.
- Finite and infinite, countable and uncountable sets.
- Cardinal and ordinal numbers. Peano arithmetic, mathematical induction.
- NBG and ZFC systems of axioms of set theory. Axiom of choice. Zorn's lemma.
- Fundamentals of symbolic computation (Mathematica).

Course name: **STATISTICS**
Number of ECTS credits: **6**

Content:
- Introduction. What is statistics? Examples of applications of statistical methods in natural sciences. Population. Sample.
- Random variables. Continuous and discrete random variables. Examples of random variables. Probability function, probability density function, cumulative distribution function.
- Descriptive statistics. Frequency distribution. Measures of central tendency. Quantiles. Measures of variability.
- Sampling. Introductory examples. Random sampling. Sampling distribution. Standard error. Confidence intervals.
- Graphical methods of data representation. Histogram. Scatter plots. Box and whisker plot. QQ-diagram.

- Hypothesis testing. Null hypothesis, alternative hypothesis. Errors in hypothesis testing. Examples: t-tests (mean of single sample, means of two independent/dependent samples, ANOVA)
- Correlation and dependence. Regression. Linear regression. Measures of linear dependence. Correlation coefficients. Non-linear dependencies. Association, contingency tables.

Course name: **ORGANIC CHEMISTRY AND BIOCHEMISTRY**
Number of ECTS credits: **6**

Content:
Students in the course acquainted with the basics of organic chemistry. They gain knowledge of the structure, property and the role of specific organic compounds and their reactivity. Students deepen their knowledge of various types of organic compounds, their structure, reactivity and the possibility of transformation of one organic compounds in the other with focusing on the functionalization of organic compounds. Gain a basic knowledge in the field of organic chemistry, which will serve as the basis for the acquisition of new science knowledge especially in biochemistry. Students learn about the structure, function, biosynthesis and degradation of the major life biomolecules, especially proteins and enzymes. Are able to identify, isolate and quantified biomolecules. Proficient in many techniques, methods and apparatus which are necessary for this. At the same time get insight into the dynamic process of metabolism, the key metabolites in individual metabolic cycles and their interconnection in regulatory mechanisms that maintain cells in a steady state.
If the balance in the cell breaks down for various reasons, it may be a variety of metabolic diseases.

Course name: **ALGORITHMS IN BIOINFORMATICS**
Number of ECTS credits: **6**

Content:
- Introduction to bioinformatics, basic bioinformatics problems in molecular biology, brief biological introduction.
- Algorithms for sequence analysis: based on pattern searching, sliding windows, matrices, classical statistical methods and graphical presentations.
- Comparison of two sequences: algorithms for exact matching.
- Comparison of two sequences: heuristics algorithms.
- Pattern matching and finding the best match.
- Suffix trees.
- Comparison of multiple sequences.
- Construction of evolutionary trees.
- Similarity search: problem definition, matrices, methods.
- Aligning two or more sequences: problem definition and methods, 2-approximation algorithm for multiple sequence alignment with respect to sum-of-squares distance function.
- Phylogenetic analysis: distance calculation, parsimony methods, maximum likelihood methods, bootstrapping, perfect phylogeny and extensions, Gusfield's algorithm for binary matrices. Modeling of the perfect phylogeny problem with chordal graphs.

Course name: **SYSTEMS II – OPERATING SYSTEMS**
Number of ECTS credits: **6**

Content:
- Introduction: what is operating system, history of operating systems, computer hardware overview, concepts of operating systems, system calls, operating system structure.
- Processes and threads: processes, threads, inter-process communication, critical conditions, critical region, classical IPC problems, scheduling.
- Deadlocks: resources, representation of processes and resources, deadlock modeling, Osterich algorithm, deadlock detection and recovery, deadlock avoidance, deadlock prevention.

- Memory: basic operations, swapping, virtual memory, page replacement algorithms, modeling page replacement algorithms, page management system, segmentation, Multics, Pentium.
- Input/output: principles of I/O hardware, principles of I/O software, software levels of I/O, disk, clock, character terminals, graphical interfaces, network terminals, other I/O equipment.
- File systems: files, directories, file system implementation, examples of file systems – Unix, Windows.
- Multimedia: multimedia files, video compression, JPEG, MPEG, scheduling multimedia processes, multimedia file systems, storing multimedia files, disk scheduling.
- Multi-processor systems: multi-computer systems, distributed systems, architectures and examples.
- Security: security environment, introduction to cryptography, user authentication, attacks from inside, attacks from outside, protection mechanisms, trusted systems.
- Unix-Linux: history of UNIX, overview of UNIX, UNIX processes and memory management, UNIX I/O and file system, UNIX security.

Course name: **DATA STRUCTURES AND ALGORITHMS**
Number of ECTS credits: **6**

Content:
- The basic mathematical tool
- Basic data structures
- The basic abstract types and their performance
- Sorting and frineds:
- Basic algorithmic techniques
- Algorithms on graphs and networks
- Selected algorithms

Course name: **INTRODUCTION TO DATABASE SYSTEMS**
Number of ECTS credits: **6**

Content:
The course will cover topics that might include (but are not restricted to) any of the following according to the needs and development of the subjects covered:
- Introduction
- Entity-Relationship model
- Relational model
- Relational algebra and calculus
- SQL and QBE
- Disks and files
- Indexes
- Evaluation of relational operations
- Query optimization
- Transactions
- Concurrency control and crash recovery
- Database design

Course name: **DATA PROGRAMMING**
Number of ECTS credits: **6**

Content:
1. Introduction to data programming.
Programming languages for data programming, basic data structures and operations, applications.

2. Introduction to Python.

Interpreter environement, syntax, numbers, strings, lists, files, sequential control, loop control, functions, lambda expressions, higer-order functions, functional programming.

3. Data structures in Python.
Lists, products, sequences, sets, dictionaries, loops for data structures.

4. Modules and classes in Python.
Syntax of modules, module environment, standard modules, syntax of classes, classes as objects, instances, methods, inheritance, itarators, generators.

5. Numeric Python (numpy).
N-dimensional arrays, indexes and array slicing, operations, data processing, data cleaning, data transformations, aggregations, grouping, timeseries, structured arrays.

6. Basics of R programming language.
History of R. Characteristics of R programming language, usage, graphical user interfaces for R, R studio - how it looks like and how it works, basic usage of command-line interface (practical example), numbers, vectors, R commands, functions and definitions, objects, attributes, matrices, lists, factors, data frames.

7. Reading and writing in R.
Reading of objects, vectors and matrices, reading data frames, reading from files, data generating, writing R objects, writing own simple functions in R.

8. Data managing in R.
databeses, statistical models in R, graphical procedures, practical example of statistical model and graphic display usage.
9. Example of application in R.
Bioconductor, practical example of R usage in reasearch.

COMPULSORY COURSES OF THE 3RD YEAR OF STUDY

Course name: **BASIC POPULATION GENETICS**
Number of ECTS credits: **3**

Content:

- Introduction to population genetics
- Genetic and phenotypic diversity (maintenance of genetic diversity, allele frequencies, genotype frequencies, heterozygosity)
- Molecular methods and sampling in population genetics
- Genome types (nuclear, chloroplast, mitochondrial), RFLP markers, SNP, AFLP, RAPD, SSR.
- Evolutionary factors and their effects on genetic structure of populations: natural selection, mating, fragmentation of populations, migration (random mating, inbreeding, inbreeding depression, inbreeding coefficient, heterozygosity within populations, Wright's F statistic, models of migration)
- Parameters of genetic diversity
- Hardy-Weinberg equilibrium Linkage Disequilibrium analysis, causes of disequilibrium
- Random gene flow (genetic drift), Wright-Fisher model, inbreeding
- Irreversible and reversible mutation, influences on random gene flow, probability of fixation of new neutral mutations
- Genetic structure of populations (diversity, distribution of diversity between populations, genetic distances), population size, gene flow, reproduction, natural selection
- Molecular population genetics (sequence divergence, amino acid substitutions, nucleotide substitutions and their models, molecular clock), intraspecific polymorphism, polymorphism and divergence of non-coding regions, local recombination rates
- The use of population genetics in species conservation
- The use of statistical methods in population genetics

Course name: **EVOLUTIONARY GENETICS**
Number of ECTS credits: **6**

Content:
The aim of this course is to introduce students to the basic concepts of evolutionary genetics and deepen their knowledge about the usefulness of molecular tools determining evolutionary history of species. Students will acquire more detailed insight into the molecular basis of variability of living things, patterns and mechanisms of change of biological macromolecules, molecular phylogenetics, and gene evolution. Other acquired competences relate to a synoptic knowledge of evolutionary theory and mathematical representation of basic microevolutionary events. Students will be able to understand specifics of molecular evolution and application of bioinformatics into molecular evolution and phylogenetics. Lectures will provide theoretical knowledge, which will be upgraded in the tutorials with practical computational exercises and case-studies. By addressing key problems in the course the students will learn different research methods and techniques that will allow them to acquire new skills and develop critical thinking.

Course name: **STRUCTURES OF BIOLOGICAL MOLECULES**
Number of ECTS credits: **3**

Content:
The first part of the course will be focused on an introduction to classes of biological molecules with subsequent presentation of more complex biological molecules.

Then, experimental methods important for protein 3D structure determination will be introduced, especially protein crystallography and protein NMR.

In the course also theoretical methods for 3D structure prediction such as homology modelling fold recognition method and ab initio methods will be presented. A review will be provided of main available databases and analytical tools for studying biological molecules.

Finally, students will familiarize themselves with the utilization of computational chemistry for studying structure of biological molecules and its utilization in drug design.

In the scope of the practical sessions of the class these themes will also be examined in the computer classroom with several examples.

Major themes:
- overview of biological molecules,
- determination of 3D protein structures: protein crystallography, protein NMR spectroscopy,
- theoretical predictions of 3D structures of proteins,
- databases of biological molecules and their use (PDB, SCOP2, CATH, CSD, Expasy, GeneCards, UniProt, KEGG),
- introduction to molecular modeling and utilization of computational tools for studying protein structure and drug design (selected examples).

Course name: **SYSTEMS III – INFORMATION SYSTEMS**
Number of ECTS credits: **6**

Content:
Modern society is based on information management, which enables it to more quickly adapt to changes in needs and requirements. Computer aided information systems play the key role in this process. This course deals with their influence on the business environment as well as with their design and development.
The course will cover topics that might include (but are not restricted to) any of the following according to the needs and development of the subjects covered:
- Basic definitions and the role of information systems in information society.
- Information systems in business process.

- Systems development life cycle (SDLC).
- Systems analysis and design, structured and object-oriented approach.
- Data and process models and diagraming techniques. Data dictionary, structure diagram, DFD, ER, ELH. Introduction to UML.
- Collecting information, traditional and modern techniques.
- Interface design, service oriented architecture (SOA).
- Cloud computing.

Course name: **MATHEMATICAL MODELLING**
Number of ECTS credits: **6**

Content:
- *Introduction.* What is mathematical modeling? The role of mathematical models in natural sciences and economics. Types of mathematical models.
- *Programming tools*. A short overview of Octave/Scilab.
- *Optimization.* Critical point, minimum, maximum, saddle. Taylor's formula for scalar fields. Local extrema and local extrema under constraints. Newton's method. Applications: discrete catenary, truss stability etc.
- *Calculus of variations.* Standard problem of variation calculus. Isoperimetric problems. Applications: catenary, brachistochrone, truss oscillations, etc.
- *Linear programming*. What is a linear program? Examples of linear programs: optimal diet, flow in a network etc. Forms of linear programs. The fundamental theorem of linear programming. Simplex method. Duality. Integer linear programming and LP relaxation. Applications.
- *Differential equations and systems of differential equations as mathematical models in natural sciences*. Motivational examples. Equilibrium. (Linear) Stability of equilibria. Phase portraits. The basics of Poincare-Bendixon theory. The basics of bifurcation theory. Applications: epidemic models, models of competition, models of symbiosis, predator-prey dynamics, molecular kinetics, basic neurological models, models in economics.

Course name: **MATHEMATICAL MODELLING IN BIOINFORMATICS**
Number of ECTS credits: **6**

Content:
- *Introduction.* What is mathematical modeling? The role of mathematical models in natural sciences. Types of mathematical models.
- *Programming tools*. A short overview of Octave/Scilab.
- *Differential equations and systems of differential equations as mathematical models in natural sciences*. Motivational examples. Equilibrium. (Linear) Stability of equilibria. Phase portraits. The basics of Poincare-Bendixon theory. The basics of bifurcation theory. Applications: epidemic models, models of competition, models of symbiosis, predator-prey dynamics, molecular kinetics, basic neurological models.

Course name: **BIOINFORMATICS PRACTICE**
Number of ECTS credits: **6**

Content:
In this course we will learn bioinformatics approaches and tools in the field of genomic data. In the introductory part, we will learn the basics of molecular biology with an emphasis on genes, transcripts and proteins, and their functions and interactions. Modern molecular biology techniques enable us to carry out measurements of a large number of genes and/or proteins simultaneously. We will learn approaches that are adapted for the analysis of high-density omics data focusing on the level of gene expression. We will wrap up the subject with a seminar by applying the presented methods on real-world data from studies of molecular mechanisms and diseases, such as immune response and metabolic syndrome.
- Introduction: basis of molecular biology, omics studies and biotechnology

- Biological databases and data analysis tools
- Analysis of high-throughput omics data
- Molecular evolution of human gene

Course name: **PHYSICAL CHEMISTRY WITH CHEMINFORMATICS**
Number of ECTS credits: **6**

Content:
- Gasses and intermolecular forces : the ideal gas, kinetic theory of gases, intermolecular interactions, the van der Waals gas
- Energy: the first law of thermodynamics, changes of internal energy and enthalpy in physicochemical processes, thermochemistry
- Entropy: the second law of thermodynamics, entropy of gasses and gas mixtures, entropy changes in physicochemical processes, the third law of thermodynamics
- Biomolecular simulations: topology of biomacromolecules, protein data bank, force-field parameters, solvation and ionic atmosphere, energy minimization and molecular dynamics
- Structural analysis of trajectories: radial pair-distribution functions of ions, root-mean-square deviation of structure, root-mean-square fluctuation of structure, radius of gyration, heat-to-tail distance, hydrogen-bond analysis, conformational clustering
- Energy analysis with free energy: van der Waals and electrostatic interaction, energy decomposition
- Visualization of simulation trajectories and biomolecular computer graphics

ELECTIVE COURSES

(Read the short descriptions of all elective courses of the study programme. In the table Elective courses you will find the list of the elective courses which were offered in the last two years.)

Course name: **BIOMOLECULAR MODELING**
Number of ECTS credits: **6**

Content:
Students will familiarize themselves with 3D macromolecular modelling from the available experimental data.
Major themes:
- macromolecular modeling by using crystal and NMR structures
- application of force fields in modeling and refinement of 3D structures
- dynamic characteristics of macromolecules, application and comparison of molecular dynamics and NMA (Normal Mode Analysis)
- visualization and interpretation of 3D models
- free-energy calculations
- molecular docking
- quantum-chemical simulations
- pharmacophore and virtual screening
- QSPAR

Computer exercises: practical examples of modeling of ligand-receptor structures using programs GROMACS, bio3d, VMD, MAIN, GAUSSIAN and ProBiS.

Course name: **MATHEMATICAL CHEMISTRY**
Number of ECTS credits: **6**

Content:
A. Theoretical basis
- Basics of classical combinatorics
- Basics of formal languages
- Basics of graph theory

- Matrices, eigenvalues, eigenvectors
- Maps on surfaces, Euler formula
- Graph algorithms in Sage and Python

B. Families of molecular graphs, Applications in chemistry and biology
- Molecules and chemical graphs
- DNA, RNA as strings
- Proteins as strings of aminoacids
- Trees, molecular trees, alkanes
- Benzenoids and their generalizations
- Fullerenes and fullerene-like structures
- Cubical and subcubical graphs
- Generating graphs using tools such as CaGe
- House of Graphs and similar databases

C. Problems on graphs with applications
- Spectral graph theory (Hückel theory, HOMO-LUMO)
- Matching theory (Kekulé structures)
- Hamilton cycles
- Graph coloring (Vertices correspond to atoms)
- Euler circuits (polyhedral self-assembly)

D. Representation of graphs, graph drawing, molecular mechanics
- Graph drawing using eigenvectors
- Force-field methods
- Rotagraphs and other polycriculants

E. Graph invariants and topological indices
- Wiener index
- Szeged index
- HL index
- etc.

Each chapter is supported by programs in Sage.

Course name: **SYSTEMS BIOLOGY APPROACH IN HUMAN DISEASE STUDY**
Number of ECTS credits: **6**

Content:
In this course students will familiarize with critical parameters in modern experimental medical research.
Students will learn about developing good research questions and hypothesis, clinical studies and experimental design, variables and confounders, statistical analysis and data interpretation and presentation. The students will practice the selection of variables, consider the influence of co-variables, testing multiple hypothesis and the effect of sample size and power analysis. They will be introduced to basics of epidemiology and why it is important for human disease research, evidence based medicine and meta-analyses.
The seminar lectures will include the basics of molecular biology methods with an emphasis on presentation of data about genes, epigenetics, transcripts, proteins and metabolites and their functions and interactions. Students will practicaly use programs for analysis and graphical data presentation of data and learn on examples how to write a scientific paper or research thesis and how to make an oral research presentation. Students will learn how to answer concrete research questions in human disease. Seminar lectures will present methods on real-world data from studies of molecular mechanisms and diseases, such as immune response and metabolic syndrome.

Major themes:
- Formulating experimental question and testing hypothesis (variables- dependent, independent, co-variables, confounding; drawing conclusions-deduction, induction, comparison; validity, reliability of results-errors (type I, II, confidence interval, bootstraping), population effect size and power analysis

- Study design, *in vitro/in vivo* experiments, types of pre-clinical, clinical studies; sampling, sample size, replication, randomization; error and bias of sample, experiment performance and study design
- Conducting multiple comparisons (post hoc tests, Bonferroni, Tukey..), ANCOVA, practical use of regression, basics of epidemiology
- Biostatistic of diagnostic test and method comparison (analytical, diagnostic specificity, sensitivity, predictive value)
- Systems medicine, 4P medicine, precision medicine
- Systems medicine in research and development of new drugs
- Ethical issues, informed consent, personal information privacy
- Overview of –omic data methods and methods for their further confirmation in medical studies with emphasis on transcriptomics, proteomics and metabolomics; overview of databases and freely available tools for their analysis with cases from different diseases

Practical approaches in solving modern medical research questions:
- Each seminar lecture will focus on one of human diseases and the data gathered about it (eg rheumatoid arthritis, atherosclerosis etc)
- Experimental data obtained from genomics, epigenetics, proteomics, metabolomics will be used and their advantages/disadvantages discussed
- Using online deposited data and data bases
- Data visualization, tables and graphs for research paper/thesis and oral presentation -using program for data presentation and statistical analysis
- Students will practice study conduct to compare two study populations and think of what variables could affect the treatment outcome or disease outcome and propose possible way of obtaining those information's from study population (i.e. digital biomarkers, increased use of wearable devices provide unique opportunities to develop innovative therapeutic strategies)

Course name: **TRAINING IN THE WORKPLACE**
Number of ECTS credits: **6**

Content:
Student, according to their own interests, selects or proposes a department in the organization where they would like to get a work experience placement. The content of work experience will thus depend mainly on the chosen field of work and student's activities. It is defined jointly by both student and mentor from the organization in the work experience plan, which is confirmed by a faculty coordinator.

Work experience plan includes description of a problem and goals of a project in which the student is about to participate as well as the students assignments.

As INTERNALLY ELECTIVE COURSES students can also choose the following courses from the undergraduate study programmes at UP FAMNIT:

- **Mathmematics**: Algebra II – Linear Algebra; Introduction to Numerical Calculations; Algebra III – Abstract Algebra; Game Theory; Analysis III – Functions of Many Variables; Probability; Stochastic Processes;
- **Mathmematics in Economics and Finance**: Stochastic Processes II;
- **Computer Science:** Theoretical Computer Science II – Formal Languages and Computability; Theoretical Computer Science III - Information Theory; Systems I – Hardware; Programming III – Concurrent Programming; Computer Networks;
- **Conservation Biology:** Conservation Biology; Systematic Botany and Geobotany; Environmental Monitoring; Geographical Information Science and Use; Marine Biodiversity; Protected Areas and Sustainable Use; Biogeography; Ecotoxicology; Biodiversity and Ecology in the Mediterranean; Evolution Biology; Biological Topics in English; Ecology;
- **Mediterranean Agriculture** (higher education professional): Plant Biotechnology; Plant Molecular Diagnostic; Plant Breeding and Propagation.

Contents of the above mentioned courses are available in the presentation of the study programme (Course structure).