Specific part of the examination regulations for the consecutive Master's program "Artificial Intelligence for Molecular Sciences" at the Technische Universität Braunschweig

On 18.06.2024, the Faculty Council of the Faculty of Life Sciences, and on 20.06.2024 in urgent authorization the dean of the Faculty of Life Science adopted the following specific part of the examination regulations for the degree program "Artificial Intelligence for Molecular Sciences" with the degree "Master of Science" in addition to the general part of the examination regulations for the Bachelor, Master, Diploma and Magister degree programs at the Technische Universität Braunschweig (APO).

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§ 1 Subject Matter and Standard Period of Studies

(1) These examination regulations contain in particular the study regulations, examination modalities and other provisions for the consecutive Master's program “Artificial Intelligence for Molecular Sciences” of the Faculty of Life Sciences.

(2) The Master's degree program has a research-oriented profile.

(3) The standard period of study in which the degree can be completed is four semesters, including the Master's thesis. The range of courses and examinations offered is designed in such a way that students can obtain the Master's degree within the standard period of studies.

§ 2 University Degree and Certificate

(1) After 120 credit points required to pass the Master's examination have been acquired, the University degree “Master of Science” (abbreviated to “M. Sc.”) in the subject “Artificial Intelligence for Molecular Sciences” is awarded.

(2) A certificate will be issued in German and English in accordance with the template attached to the APO in accordance with appendix 2. In addition, a certificate and a Diploma Supplement (specific EU document) will be issued in German and English in accordance with the template attached to the APO in accordance with appendix 1 and 3.

(3) If the overall grade is 1.3 or better, the grade “with distinction” (“mit Auszeichnung”) is awarded. The grade must be stated on the certificate in addition to the overall grade.

§ 3 Structure of Studies

(1) The degree program is divided into modules. The successful completion of a module requires the successfull completion of the coursework and Examination Achievements associated with the module in accordance with appendix 4, so that the intended learning outcomes listed in appendix 3 have been achieved and the corresponding credit points have been acquired.

(2) The Master's degree program is divided into the following areas:
- Basic Area (compulsory modules, 26 credit points)
- Advanced Area (compulsory elective modules, 15 credit points)
- Profile Area (compulsory elective modules, 37 credit points)
- Key qualification area (12 credit points)
- Master's thesis (30 credit points).

The modules that can be taken in the individual areas are listed in appendix 3 and 4.

(3) The modules listed in appendix 4 must be completed for the Basic Area (Compulsory Modules). In the Advanced Area (compulsory elective modules), modules amounting to 15 CP must be completed from the modules offered (see appendix 4).

(4) In the Profile Area, students choose one of the three fields of specialization offered: “Chemical Synthesis and Drug Design”, “Spectroscopy and Imaging” and “Data-Driven Biology”. The modules offered in these fields of specialization are listed in appendix 2.

(5) In the chosen field of specialization, a basic profile module and further modules from the chosen field of specialization must be completed in accordance with appendix 2. In addition, a research internship of 12-17 CP must be completed in the chosen profile area. If full modules have been completed in excess of the required number of credit points, the modules not to be graded can be specified upon application, otherwise the assessment will be based on the order in which the modules were passed. The application must be submitted to the Examination Committee before taking the last examination required to pass the degree program.

(6) With the approval of the Examination Committee, a maximum of two modules from another field of specialization may be included in the chosen area of specialization if they complement the study plan in a meaningful way.

(7) A maximum of two modules that are not listed in the appendixes may be approved in the Advanced Area or in the Profile Area upon application to the Examination Committee (flexi-modules), provided that they complement the study plan in a meaningful way.

(8) The key qualification area consists of the module “Ethics and Epistemology” and the module “Professionalization Module” and primarily serves the acquisition of personal, methodological and social skills. It is made up of corresponding Study Achievements with interdisciplinary and action-oriented offers to impart interdisciplinary and practical professional qualifications / skills (see appendix 4).

(9) With the approval of the Examination Committee, work that contributes to the acquisition of the intended learning outcomes of the professionalization module can also be completed outside of a Master's or Bachelor's degree program at TU Braunschweig.

§ 4 Mentoring Program

Together with their assigned mentor, students draw up an individual study plan at the beginning of their studies in order to set specific study focuses. The study plan countersigned by the mentor must be submitted to the Examinations Office before the end of the lecture period of the first semester. Any necessary adjustments to the study plan during the course of studies are made jointly by the student and the mentor. The amended study plan, countersigned by the mentor, must be submitted to the Examinations Office.

§ 5 Study and Examination Achievements

(1) In addition to §9 Section 1 of the APO, the following achievements are to be assessed as Study Achievements:

a. Colloquium: A colloquium is an oral examination in the form of a discussion between the student and the lecturer, in which it is determined whether the student is prepared for one or more internship experiments and/or about the presentation and critical appraisal of the task worked on and its solution.

b. Exercises and homework: Exercises and homework are used to prepare and follow up on the content taught in the course. Students should independently practise and consolidate the concepts and methods introduced in the course using examples.

c. Protocol: A protocol contains the written presentation and critical appraisal of the task worked on and its solution.

d. Laboratory journal: Written record of all experimental results during a practical course. This also includes modifications in the material-method section, figures, tables, graphs of the raw data and their initial evaluation. A laboratory notebook is structured chronologically and the author must be clearly identified.

(2) The student's application to have the result of the graded or ungraded Study Achievement taken into account for Written Exam+ or Oral Exam+ must be submitted no later than the start of the examination.

(3) If TU Braunschweig is forced to suspend in-person examinations, e.g. due to a pandemic situation, the type of examination may be changed two weeks before the examination between a written or written+ examination and a take-home examination in accordance with §9 d APO, provided that the competences to be tested are equivalent. In these cases, the examiners are responsible for choosing the respective type of examination.

§ 6 Type and Scope of the Examinations

(1) The examination contents are derived from the intended learning outcomes of the individual modules in accordance with appendix 3, which are based on the vocational requirements which can alternatively be consulted.

(2) The language of courses and examinations is English by default. Exceptions are at the discretion of the Examination Committee.

(3) The number of credit points allocated to the module must be taken into account when determining the duration of the examination: Approximately 20 minutes are set per credit point for written final module examinations and approximately five minutes for final oral module examinations, which may also contain written elements.

§ 7 Registration and Admission to Exams

(1) Admission to the individual module examinations must be applied for online from the Examination Committee or the appointed body no later than 1 week before the examination date. Withdrawal from an examination within the meaning of §11 Section 1 of the APO must be declared in corresponding form.

(2) Attendance is mandatory in the laboratory courses as well as in the seminars preparing for and accompanying the laboratorty courses. In the event of absences, in justified individual cases (e.g. illness), proof that the required learning objective has been achieved can be provided in an appropriate form in consultation with the examiner at a later time.

(3) In accordance with §13 Section 4 of the APO, it is stipulated that in a maximum of three cases, examinations in elective and compulsory elective modules that were not passed at the first attempt outside the standard period of studies do not have to be repeated and can be discontinued.

§ 8 Special Conditions for the Master's Thesis

(1) The Master's thesis is usually completed in the 4th semester. It comprises of 30 credit points.

(2) The topic of the Master's thesis must include a research question from the field of “Artificial Intelligence for Molecular Sciences” in the broader sense and should be chosen in such a way that it matches the chosen profile area in terms of content.

(3) The Master's thesis must be written in English. The Examination Committee decides on exceptions. The application must be submitted to the Examination Committee not later than the registration of the Master's thesis. An English summary must be attached to the non-English Master's thesis.

(4) In order to be admitted to the Master's thesis, students must have demonstrably completed at least 75 credit points of coursework and examinations. In justified cases (e.g. if modules have not yet been completed for reasons for which the student is not responsible), the Examination Committee may allow exceptions to this rule upon application.

(5) Students are given the opportunity to present their Master's thesis as part of the working group or institute seminar.

§ 9 Supplementary Examinations

(1) Deviating from §18 section 1 sentence 2 of the APO, the application for assessment as a supplementary examination may also be submitted after the coursework or examination has been completed, but no later than the day on which the last coursework or examination required for successful completion of the degree program was completed.

(2) In accordance with §18 section 1 sentence 7 APO, it is stipulated that passed examinations in elective and compulsory elective areas can be replaced by supplementary examinations, provided that these correspond in content and scope to the examinations to be replaced. The application must be submitted to the Examination Committee before taking the last examination required to pass the degree program.

§ 10 Part-time studies

The degree program is suitable for part-time study in accordance with the TU Braunschweig matriculation regulations.

§ 11 Entry into Force

These examination regulations enter into force on 01.10.2024.

Appendix 1 - Program-specific components of the Diploma Supplement (specific EU document)

2.1 Bezeichnung der Qualifikation (ausgeschrieben, abgekürzt)
Master of Science (M. Sc.)

2.2 Hauptstudienfach oder –fächer für die Qualifikation
Artificial Intelligence for Molecular Sciences

2.5 Im Unterricht / in der Prüfung verwendete Sprache(n)
Englisch, in einigen Fällen Deutsch

3.1 Ebene der Qualifikation
Master-Studium, forschungsorientiert
weiterführender Hochschulabschluss

3.2 Dauer des Studiums (Regelstudienzeit)
Zwei Jahre (inkl. schriftlicher Abschlussarbeit), 120 ECTS Leistungspunkte

3.3 Zugangsvoraussetzung(en)
Bachelorabschluss oder gleichwertiger Abschluss in Chemie, Lebensmittelchemie, Biologie, Biotechnologie oder in einem anderen fachlich geeigneten Studiengang

4.1 Studienform
Vollzeitstudium

4.2 Anforderungen des Studiengangs/Qualifikationsprofil des Absolventen/der Absolventin
Im Masterstudiengang „Artificial Intelligence for Molecular Sciences“ (AIMS) erwerben die Studierenden eine vertiefte wissenschaftliche Ausbildung und die Fähigkeit zum selbstständigen wissenschaftlichen Arbeiten. Die Studierenden werden in datengestützten Methoden sowie in Methoden der künstlichen Intelligenz ausgebildet und zur Anwendung dieser Methoden in den molekularen Wissenschaften befähigt werden. Zur Profilbildung werden drei Anwendungsprofile „Chemical Synthesis and Drugs“, „Spectroscopy and Imaging“ sowie „Data-Driven Biology“ angeboten.

Durch den Schlüsselqualifikationsbereich erwerben die Studierenden Zusatzqualifikationen. Sie können aus Veranstaltungen wählen, die z. B. Sprachkompetenz, Sozialkompetenz, Projektmanagement und fremde Fachkulturen vermitteln. Durch die abschließende Masterarbeit, für deren Bearbeitung sechs Monate vorgesehen sind, wird die Befähigung zu eigenständiger wissenschaftlicher Arbeit nachgewiesen.

Die Absolvent:innen des Masterstudiengangs „Artificial Intelligence for Molecular Sciences“ (AIMS)

- sind in der Lage, Datensätze in den molekularen Wissenschaften zu erheben, zu kuratieren, zu analysieren und zu visualisieren.
- können datengestützte Analysemethoden und Algorithmen der künstlichen Intelligenz für verschiedene Fragestellungen kompetent auswählen, kombinieren, und ggf. anpassen und weiterentwickeln.
- können Forschungssoftware für ausgewählte Anwendungen nachhaltig entwickeln.
- besitzen vertiefte Spezialkenntnisse in mindestens einem Spezialgebiet der molekularen Wissenschaften.
- sind in der Lage, datengestützte Methoden und Methoden der künstlichen Intelligenz für Anwendungen in den molekularen Wissenschaften auszuwählen und diese selbstständig anzuwenden, um Probleme zu analysieren und ggf. zu lösen.
- sind in der Lage, wissenschaftliche Publikationen zu verstehen und die darin beschriebenen Methoden in der eigenen Arbeit umzusetzen.
- sind in der Lage, selbstständig eine wissenschaftliche Problemstellung zu lösen und dafür wissenschaftliche und technische Daten zu erarbeiten, interpretieren, bewerten und fundierte Urteile abzugeben, die wissenschaftliche, technologische und ethische Aspekte berücksichtigen.

2.1 Name of Qualification (full, abbreviated; in original language)
Master of Science (M. Sc.)

2.2 Main Field(s) of Study
Artificial Intelligence for Molecular Sciences

2.5 Language(s) of Instruction/Examination
English, in some cases German

3.1 Level
Master' s degree (graduate/second degree), by research with thesis

3.2 Official Length of Programme
Two years (120 ECTS credits)

3.3 Access Requirements
Bachelor degree or similar degree in Chemistry, Food Chemistry, Biology, Biotechnology or in thematically related field

4.1 Mode of Study
Full-time

4.2 Programme Requirements/Qualification Profile of the Graduate

The Masters programme „Artificial Intelligence for Molecular Sciences“ (AIMS) Chemistry provides the students with an advanced scientific education and with the ability to undertake independent scientific investigations. The students are educated in data-driven methods as well as methods of artificial intelligence and are able to apply such methods in the molecular sciences. For specialization, the three profile areas “Chemical Synthesis and Drugs“, “Spectroscopy and Imaging“, and “Data-Driven Biology“ are offered.

Courses on key competences gives students the chance to acquire additional qualifications. They can choose between courses that offer e. g. foreign languages, social skills, project management or insights into completely different branches of scientific culture. To complete their studies, the students have to write a Master’s Thesis, for which 30 ECTS points are awarded. During their six-months Master project, the students demonstrate their ability to carry out independent scientific research.

The Graduates of the Master Study Course „Artificial Intelligence for Molecular Sciences“ (AIMS)

- are able to curate, to analyze, and to visualize data sets in the molecular sciences.
- can select, combine and, when necessary, adapt and improve data-driven methods and algorithms of artificial intelligence for different.
- can develop scientific software for selected applications in a sustainable fashion.
- have specialized knowledge in at least one area of the molecular sciences.
- are able to select and independently apply data-driven methods and methods of artificial intelligence for applications in the molecular sciences for analyzing and possibly solving scientific problem.
- are able to read and understand scientific publications and to incorporate the corresponding methods into their work.
- are able to solve scientific problems on their own and, to this end, collect scientific and technical data, analyze them and draw conclusions that take into account scientific, technological and ethic aspects.

- sind in der Lage, ihre wissenschaftliche Arbeit mündlich und schriftlich zu diskutieren und eine wissenschaftliche Publikation zu verfassen.
- können erfolgreich interdisziplinär in einer Gruppe arbeiten und können ihre erarbeiteten wissenschaftlichen Ergebnisse angemessen darstellen und diskutieren.
- können effizient mit Fachvertreter:innen und mit anderen Zielgruppen kommunizieren.
- sind damit befähigt, eine wissenschaftliche Tätigkeit mit dem Ziel einer Promotion auszuüben.

4.3 Einzelheiten zum Studiengang
Einzelheiten zu den belegten Kursen und erzielten Noten sind im Zeugnis enthalten, gleiches gilt für das Thema und die Bewertung der Abschlussarbeit. Einzelheiten zu möglichen Auslandsaufenthalten
- zu Studienzwecken siehe Transcript of records der Gasthochschule oder Vergleichbares
- zu Praktikumszwecken siehe Praktikumszeugnis oder Vergleichbares
- zu Forschungszwecken siehe Forschungsbericht oder Vergleichbares

4.4 Notensystem und Hinweise zur Vergabe von Noten
Allgemeines Notenschema (Abschnitt 8.6):

1,0 bis 1,5 = „sehr gut“
1,6 bis 2,5 = „gut“
2,6 bis 3,5 = „befriedigend“
3,6 bis 4,0 = „ausreichend“
Schlechter als 4,0 = „nicht bestanden“

1,0 ist die beste Note. Zum Bestehen der Prüfung ist mindestens die Note 4,0 erforderlich.
Ist die Gesamtnote 1,3 oder besser, wird das Prädikat „mit Auszeichnung“ vergeben. Die Gesamtnote ergibt sich aus den nach Leistungspunkten gewichteten Einzelnoten.
ECTS Note: Nach dem European Credit Transfer System (ECTS) ermittelte Note auf der Grundlage der Ergebnisse der Absolventinnen und Absolventen der zwei vergangenen Jahre: A (beste 10 %), B (nächste 25 %), C (nächste 30 %), D (nächste 25 %), E (nächste 10 %)

6.1 Weitere Angaben
Entfällt

6.2 Informationsquellen für ergänzende Angaben
www.tu-braunschweig.de
www.tu-braunschweig.de/flw

- are able to present and discuss their own scientific results orally and in writing and are able to write a scientific publication.
- can work in interdisciplinary teams and are able to present and discuss their scientific results adequately.
- are able to communicate efficiently with representatives of their own subject and with other target groups.
- are thus able to pursue an advanced scientific research project with the goal of obtaining a Doctorate.

4.3 Programme Details
Details of courses taken and grades achieved are included in the certificate (“Zeugnis”); the same applies to the topic and the grading of the final thesis.
Information regarding possible stays abroad during studies
- for study purposes, see transcript of records or equivalent documents
- for internship purposes, see internship certificate or equivalent documents
- for research purposes, see research report or equivalent documents

4.4 Grading System
General grading scheme (Sec. 8.6):

1.0 to 1.5 = “excellent”
1.6 to 2.5 = “good”
2.6 to 3.5 = “satisfactory”
3.6 to 4.0 = “sufficient”
Inferior to 4.0 = “non-sufficient”

1.0 is the highest grade, the minimum passing grade is 4.0.
In case the overall grade is 1.3 or better the degree is granted “with honors”.
The overall grade is the average of the student’s grades weighted by the number of credits given for each course.
In the European Credit Transfer System (ECTS) the ECTS grade represents the percentage of successful students normally achieving the grade within the last two years: A (best 10 %), B (next 25 %), C (next 30 %), D (next 25 %), E (next 10 %)

6.1 Additional Information
Not applicable

6.2 Further Information Sources
www.tu-braunschweig.de
www.tu-braunschweig.de/flw

Appendix 2 - Assignment of modules to the fields of specialization

Field of specialization "Chemical Synthesis and Drug Design" (37 LP)

Module offer in the areas of specialization "Chemical Synthesis and Drugs"		**LP**
AM-A-1 Reaction Mechanisms	Basic profile module	4
AM-A-2 Organometallic Chemistry	Basic profile module	4
AM-A-3 Catalysis		8
AM-A-4 Advanced Inorganic Chemistry		8
AM-A-5 Organic Synthesis Planning		4
AN-A-6 Enzyme Engineering		10
AM-A-7 Fundamentals of Protein Structure Analysis		10
AM-A-8 Biomolecular Modelling		8
AM-A-9 Advanced Theoretical Chemistry		8
AM-A-10 Machine Learning in Computational Chemistry		8
AM-A-RP Forschungspraktikum „Chemical Synthesis and Drug Design"		13-17

In the field of specialization "Chemical Synthesis and Drugs", one of the two basic profile modules (4 CP) must be completed (compulsory module). In addition, further modules amounting to 16 - 20 CP and a research internship of 13 - 17 CP must be completed.

Field of specialization "Spectroscopy and Imaging" (37 LP)

Module offer in the areas of specialization "Spectroscopy and Imaging"		**LP**
AM-B-1 Molecular Spectroscopy	Basic profile module	5
AM-B-2 Biophysical Chemistry		8
AM-B-3 Modern Optical Methods und Imaging		8
AM-B-4 Solar and Chemical Energy Conversion		8
AM-B-5 Physical Biology of the Cell		10
AM-B-6 Sophisticated Imaging		10
AM-B-7 Chemometrics		6
AM-B-8 Theoretical Spectroscopy		8
AM-A-10 Machine Learning in Computational Chemistry		8
AM-B-RP Forschungspraktikum „Spectroscopy and Imaging"		12-16

In the field of specialization "Spectroscopy and Imaging", the basic profile module (5 CP), further modules of 16 - 20 CP and a research internship of 12 - 16 CP must be completed.

Field of specialization "Data-Driven Biology" (37 LP)

Module offer in the areas of specialization "Data-Driven Biology"		**LP**
AM-C-1 Molecular Microbial Evolution and Diversity	Basic profile module	10
AM-C-2 Immunometabolism		10
AM-C-3 Comparable Quantitative Measurements and Metabolomics Biomarker Signature to Predict Case and Control		7
AM-C-4 Network Biology		5
AM-C-5 Molecular Phylogenetics and Taxonomy		10
AM-C-6 Data Literacy and Genome Research		10
AM-C-7 Applied Plant Transcriptomics		10
AM-C-8 Functional Genomics in Infection Biology		10
AM-C-9 Microbial Proteomics		10
AM-C-RP Forschungspraktikum „Data-Driven Biology"		12-17

In the field of specialization "Data-Driven Biology", the basic profile module (10 CP), further modules with a modules of 10 - 15 CP and a research internship of 12 - 17 CP must be completed.

Appendix 3 – Intended Learning Outcomes of the Modules

Basic area

Introduction to AIMS

Students have an overview of current topics and challenges in the research field "Artificial Intelligence in Molecular Sciences". They are familiar with different types of research data generated in the molecular scienc-es and are able to carry out simple analyses of such data sets. They are familiar with the methods and tools of research data management in the molecular sciences.

Mathematics for Engineers A

Students combine the mathematical methods they have learned in univariate analysis and linear algebra to describe and analyze applied problems from the technical sciences. They select and apply suitable calculation and proof methods for dealing with the mathematically formulated fundamentals of applied and technical sciences. In addition, students explain the mathematical concept formation and justify their motivation from the applications and from the mathematical concept specification and delimitation. They reproduce and explain basic proofs and proof ideas of analysis and linear algebra, and they are able to independently identify and check connections between the concepts they have learned. Students are able to analyze mathematical problems from Engineering Mathe¬matics A and the applications in technical subjects, to work out and solve treatable sub-questions and to recognize further difficulties. Finally, students will be able to use modern technical tools to solve mathematical problems.

Programming in Python and Python Lab

After successful completion of this module, students will have the competence to apply Python for de-signing and implementing small to medium software projects and analytic workflows with a focus on statistics and machine learning. During an interactive learning phase during which the students will be able to apply common packages such as scikit-learn, and they will be able to synthesize analysis work-flows for diverse data science questions. These workflows will be presented and discussed in a mini-conference among the students. After the mini-conference, students will form small teams to develop data science software tools which will be presented during the closing event. They will gain the compe-tence to critically evaluate machine learning work-flows.

Scientific Software Engineering – Lab

Students are able to develop sustainable software solutions in the scientific contexts for moderately complex engineering problems using advanced design and implementation approaches. Furthermore, they will be able to evaluate software designs with respect to various quality aspects and to make inde-pendent design decisions and implement corresponding solutions.

Advanced Area

Introduction to Machine Learning

With successful completion of the module, the students possess the following knowledge and capabilities. They are able to

- understand and correctly apply basic concepts of machine learning.
- analyse and formalize a machine learning problem.
- distinguish between typical machine learning methods.
- select a suitable method for a learning problem.
- compare and judge machine learning methods wrt their capacity.
- implement machine learning methods and apply them practically apply and parametrise respective tools.
- judge strength and weaknesses of machine learning in applications.
- recognize ethical issues in the application of machine learning.

Pattern Recognition

Upon completion of this module, students gain fundamental knowledge about methods and algorithms for classification of data. They are capable to select the appropriate means for real-world problems, to design a solution and to evaluate it.

Computer Lab Pattern Recognition

In this course, students acquire the competencies to independently select and apply appropriate machine learning and deep learning methods for complex problems. The students ...

- master the programming language Python as well as the basics of the deep learning libraries PyTorch and Tensorflow.
- evaluate the effectiveness of simple machine learning models and neuronal networks for classification and regression problems.
- evaluate the quality of deep learning models on appropriate data (sub)sets with meaningful metrics.
- know and use different types of neural networks for problems in the areas of image processing, time series processing and generative problems.
- know and use different strategies for data preprocessing and data augmentation.
- know and use different training and regularization methods for the optimization of neural networks.
- evaluate the complexity of a neural network on the basis of various parameters.

Deep Learning Lab

The Deep Learning Lab is divided in three parts:

First, the students work themselves through an introduction to the Python programming language and all required libraries for the later experiments to obtain some basic knowledge.

Second, the students will work with certain machine learning methods which are introduced in the Pattern Recognition lecture. They acquire the competence to practically apply theoretical methods for machine learning to solve small given problems.

Third, – in the so-called Machine Learning Challenge – students are required to use their obtained knowledge to develop a machine learning system in competition with the other participating teams. Therefore, the students will be provided with data which might stem from real-world/industry applications.

In the module, students acquire the competence to independently analyze a given problem, weigh suitable solution options and methods and evaluate them in terms of their functionality. In addition, students independently develop a suitable method for solving the given challenge.

Methods of Uncertainty Analysis and Quantification

Students can formulate and name elementary rules of probability theory and different ways to describe probability distributions. They can model technical/physical systems in a stochastic way using random variables. The students are further able to apply Monte Carlo and stochastic spectral methods to quantify uncertainties and also to assess the impact and propagation of uncertainties in models through global sensitivity analysis. Moreover, they are able to evaluate the numerical efficiency of the aforementioned methods. The students are also able to outline the principles of data-driven approaches to uncertainty analysis.

Profile area A "Chemical Synthesis and Drug Design"

Reaction Mechanisms

The students understand the chemical reactivity of organic molecules and are able to apply chemical reactions specifically to modify molecules. They are able to formulate and classify the underlying organic chemical reaction mechanisms. With their help, they are able to make meaningful statements about the success of planned reaction paths from the starting molecule to the target molecule and to explain the main and by-products. The students know methods to explain reaction mechanisms and can assess and discuss their range of application and significance.

Organometallic Chemistry

Students master advanced concepts in the chemistry of metals, coordination chemistry, and organometallic chemistry. They understand the role of metals in nature and are familiar with the fundamentals of bioinorganic and bioorganometallic chemistry. They can discuss and predict the structure and properties of metal complexes using modern bonding concepts and have knowledge of the use of transition metal complexes in industrial processes. They

know the principles of homogeneous and heterogeneous catalysis and are able to combine important elementary reactions into catalytic cycles and formulate them.

Catalysis

The students master the basic principles of homogeneous catalysis and the differentiation to heterogeneous catalysis and can confidently apply the underlying elementary reactions to catalytic processes. They have an overview of the most important metal-catalyzed industrial processes as well as of current developments and modern aspects of catalysis research. The students are familiar with methods of metal-catalyzed polymer synthesis and are able to evaluate and discuss the advantages of these methods compared to classical non-catalytic methods. They are familiar with methods for the characterization of polymers as well as their fields of application and are able to evaluate these methods.

Advanced Aspects in Inorganic Chemistry

The students are able to specifically build up inorganic molecular compounds and structures and to interpret and modify them with regard to their structure-activity relationships. Their understanding of the function of inorganic compounds in the biosphere as well as in supramolecular aggregates allows the students to discuss novel model compounds, switches, magnets and catalysts based on main group- and transition metals. Unusual structural and bonding relationships are competently evaluated. Students also have knowledge of interpreting and modelling spectra of paramagnetic compounds, and apply these independently.

Organic Synthesis Planning

Based on database-assisted retrosynthetic analysis, students are able to propose multi-step synthesis sequences for complex organic compounds, especially for natural and active ingredients.

Enzyme Catalysis and Enzyme Engineering

The students know different genetic and bioinformatics methods for targeted adaptation of enzyme-specific characteristics via enzyme engineering. Starting from the amino acid sequence of an enzyme, they are able to predict mutational hotspots using computational tools, to generate corresponding mutant libraries, and to select suitable assay systems for library screening.

Fundamentals of Protein Structure Analysis

After completing this module students will be able to

- name forces that lead to the formation of the stable three-dimensional structures of proteins.
- name methods that can be used to determine three-dimensional structures and to explain their underlying physical principles.
- name the most important steps in structure determination with crystallographic methods and to explain their background.
- judge the quality of published protein structures.
- suggest subsequent experiments that utilize the information contained in three-dimensional structures.
- plan scientific projects in the field of structural biology.
- grasp the content of scientific publications in the field of structural biology.
- critically analyze the content of scientific publications in the field of structural biology.
- search, present and discuss relevant scientific content.
- contribute to controversial discussions of scientific topics.

Biomolecular Modelling

The students are familiar with modern methods for modelling the structure of biomacromolecules and for simulating their thermodynamic properties. The know empirical force field methods, methods for performing molecular dynamics simulations, as well as modern multicale simulation methods. The students are able to judge the applicability and the limitations of such methods, to choose suitable simulation methods for their own research projects and to perform, analyze, and evaluate molecular dynamics simulations.

Advanced Theoretical Chemistry

The students have acquired knowledge on modern methods of quantum chemistry. They are familiar with the foundations of important methods and possess an overview of commonly used quantum-chemical methods, their implementation in scientific software, and their use in chemistry. They are able to judge the applicability and the

limits of different quantum-chemical methods and to use choose suitable methods for their own research projects, to perform quantum-chemical calculations and to analyse, evaluate, and assess their results.

Machine Learning in Computational Chemistry

The students have acquired knowledge on modern methods of molecular machine learning and molecular artificial intelligence. They are familiar with the foundations of important methods and possess an overview of commonly used methods, their implementation, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose and apply suitable methods for their own research projects and to analyse, evaluate, and assess their results.

Research Lab "Chemical Synthesis and Drug Design"

Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area "Chemical Synthesis and Drug Design" of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.

Profile area B "Spectroscopy and Imaging"

Molecular Spectroscopy

Students understand the concept of chemical bonding on a quantum chemical basis and are able to explain the structure of molecules. They understand the influence of alternating electromagnetic fields on atoms and molecules and are able to make independent quantitative statements about the absorption and emission of light using transition dipole moments and densities. They will have a thorough theoretical understanding of the spectroscopic properties of atoms and molecules and of modern spectroscopic techniques, and will be able to plan and evaluate their use to determine molecular structures.

Biophysical Chemistry

The students know the basics of the most important physicochemical methods for the elucidation of biomolecular interactions and structures and are able to decide which modern or traditional method is most efficient to answer such biochemical questions. They know the limitations and dynamic range of these methods and the importance of structure and dynamics of biomolecules for their function. Students will be able to classify which methods are suitable for studying biomolecules and answering biomolecular questions in the different environments of industrial or basic research.

Modern Optical Methods und Imaging

Optical methods are of enormous importance for the visualization of biomolecules, their structures and dynamics. On the other hand, these methods have been developing rapidly in recent years. Students acquire fundamental knowledge of the physical background of modern optical methods in the field of biosciences for imaging and the study of molecular interactions. In addition, the latest research-related methods are presented to enable students to select the optimal methods for their research questions.

Solar and Chemical Energy Conversion

Students are able to understand and competently discuss current research and application areas of solar and chemical energy conversion. They will further be able to recognize the interactions and synergies of the topics represented and to establish interdisciplinary references. Finally, the students are able to read scientific publications in the field of solar and chemical energy conversion and to classify and evaluate experiments and calculations described therein.

Physical Biology of the Cell

After completing the module, students will be able to

- understand fundamental orders of magnitude of cellular processes and from this develop their own intuition towards the measurable framework in which biological processes take place.
- understand basic terms and concepts of biophysics in cellular and molecular biological systems.

- develop interdisciplinary approaches to specific experimental problems from the quantitative methods learned in cell biophysics.
- deal intensively with data analysis up to the generation of computer models. Apply quantitative methods to cell biological preparations, analyze structures and kinetics and make predictions based on biophysical models.
- measure and analyze the function of specific cellular components.
- document, analyze and critically discuss their own results.

Sophisticated Imaging

After completing the module, students will be able to

- apply basic and advanced knowledge of modern light microscopy (LM), fluorescence microscopy, photo-manipulation and electron microscopy (EM) to their scientific questions.
- understand which relevant questions in the life sciences they can best work on with which imaging or analysis method.
- recognize and assess the advantages and disadvantages of a method.
- recognize what new insights can be gained by combining imaging methods with different resolution and magnification ranges (cross-technology) (correlative microscopy).
- present and discuss scientific content.
- engage controversially with scientific topics and issues in a group discussion.

Chemometrics

Knowledge, understanding and application of chemometric methods to pharmaceutical engineering. Critical evaluation of the performance of chemometric methods in practice.

Theoretical Spectroscopy

The students have acquired knowledge in time-dependent quantum mechanics and on modern methods of theoretical spectroscopy. They are familiar with the foundations of important methods and possess an overview of commonly used quantum-chemical methods in theoretical spectroscopy, their implementation in scientific software, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose suitable methods for their own research projects, to perform calculations and to analyse, evaluate, and assess their results.

Research Lab “Spectroscopy and Imaging”

Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area “Spectroscopy and Imaging” of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.

Profile area C "Data-Driven Biology"

Molecular Microbial Evolution and Diversity

After completing the module, students are able to

- determining and interpreting microbial diversity based on high throughput sequence datasets.
- analyzing microbial functional diversity by culture-independent approaches (including field methods).
- cultivating and isolating bacterial strains from complex communities, determining their 16S rRNA gene sequences and evaluating the taxonomy of the isolates.
- characterizing bacterial isolates by physiological and chemotaxonomical methods.
- conducting phylogenetic analyses and interpreting their results.
- interpreting morphological, physiological, and phylogenetic diversity in the context of existing information from genome sequence.
- quantifying mutation rates and interpret their implications for bacterial evolution.
- elucidating the role of accessory genes under natural conditions (by plasmid curing, competition experiments).
- integrating heterogenous datasets from own experiments, literature searches and bioinformatic analysis.
- contextualize the integrated data considering the actual state of scientific knowledge.

Immunometabolism

After completing the module, students are able to

- explain the importance of the metabolism of immune cells during infection/inflammation.
- apply modern analytical techniques, such as isotope labelling, mass spectrometry and metabolic flux analysis - evaluate and interpret GC-MS data.
- interpret the energy metabolism by means of respiration measurements.
- develop concepts for solving systems biology problems with the help of different methods.
- present and discuss scientific work.
- discuss controversial scientific topics and questions.

Comparable Quantitative Measurements and Metabolomics Biomarker Signature to Predict Case and Control

After completing the module, students are able to

- perform a simple crossover intervention study and collect samples.
- perform metabolome analyses of human saliva and/or blood samples by mass spectrometry.
- analyze the raw data with the help of bioinformatics to determine quantitative and semi-quantitative metabolite concentrations.
- identify biomarker signatures by application of machine learning algorithms (logistic regression, lasso (least absolute shrinkage and selection operator).
- quantify selected biomarkers with high precision and reproducibility.
- apply basic concepts of metrology and standardization.
- perform statistical analyses in R.
- understand the relevance of standardization for experimental design and performance.
- understand the concept of a clinical crossover study / trial to evaluate the efficacy or effects of a drug.

Network Biology

After successful completion of this module, students will have a basic understanding of graph theory and its applications for the analysis of biomedical data. They will be able to use network biology tools and critically assess network analyses. They will be capable to devise new graph-based strategies for the analysis of biomedical data.

Molecular Phylogenetics and Taxonomy

After completing the module, students will be able to

- sequence DNA using the Sanger method and review and align sequence chromatograms.
- explain and understand the methodological foundations of systematics and phylogenetic reconstruction primarily using molecular features.
- theoretically understand the basic principles of phylogenetic analysis (Maximum Parsimony, Maximum Likelihood, Bayesian Inference, and other methods) and practically apply relevant bioinformatic software.
- search DNA databases and use them for sequence comparison (BLAST).
- conceptually and practically delimit species based on molecular genetic evidence.
- independently conduct a research project, from organizing practical laboratory work to documenting data, bioinformatic analysis, interpretation, and presenting the results.

Data Literacy and Genome Research

After completing this module students will be able to

- use online resources to find and retrieve genomic information.
- work with different biological databases and data types.
- plan their own sequencing project and workflow.
- extract the genetic material needed for nanopore sequencing.
- perform long read sequencing using a portable MinION.
- work in a terminal on Linux operating systems.
- install bioinformatics tools.
- utilize latest bioinformatic tools for long read analyses.
- analyse and visualise big data.
- work in a cloud-based environment.
- critically interpret the results and summarize these in a scientific report.
- give constructive criticism during of a peer-review process.
- give a scientific talk in front of an international audience.
- communicate the results of a big data project to different target audiences.

Applied Plant Transcriptomics

After completing this module students are able to

- design experiments to study gene expression and
- conduct de novo transcriptome assembly.
- perform a quality control on RNA-seq data sets.
- analyze gene expression based on RNA-seq.
- perform functional annotations with the application of transcriptome annotation tools.
- create heatmaps and graphs using R.
- create phylogenetic trees.
- interpret the results of RNA-seq experiments.
- recognize flawed publications.
- to present and discuss scientific publications.
- to address controversial scientific topics and questions

Functional Genomics in Infection Biology

After completing this module students are able to

- understand the concepts of functional genomics. In particular, they will be able to recognise the potential and limitations of molecular genetic methods and OMICs technologies in basic and applied research and medical diagnostics.
- apply a wide range of infection genetics and functional genomics techniques to study host-pathogen interactions.
- design experiments to comprehensively answer a scientific question.
- critically analyse the advantages and disadvantages of a method and the results obtained.
- place results in a scientific context.
- present and discuss researched scientific content.
- discuss controversial scientific topics and issues in a group discussion.

Microbial Proteomics

After completing the module, students are able to

- describe the basic principles of proteomic methods and critically evaluate the advantages and disadvantages of the methods.
- identify and quantify proteins from complex protein mixtures.
- analyse large data sets and visualise the results.
- design experiments to comprehensively answer a scientific question.
- critically analyse the advantages and disadvantages of a method and the results obtained.
- place results in a scientific context.
- present and discuss researched scientific content.
- discuss controversial scientific issues in a group.

Research Lab “Data-Driven Biology”

Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area “Data-Driven Biology” of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.

Key qualification area

Ethics and Epistemology

The course:

- provides a philosophical framework and moral compass for guiding the judgement of students regarding data science and its applications (artificial intelligence, robotics, etc.).
- aims to develop communication skills, social and civic competences.
- reassures students on the limits of machines, machinery settings and machine ethics.
- strengthens personal development in the light of digit(al)ization and related claims of social change.

The students will be able to recognize and interpret social and technical problems in technology and information processing based in classical and recent position in theoretical and practical philosophy. They will be able to interpret these problems ethically and support their position with arguments from machine ethics.

Key Qualifications

The learning outcomes of the interdisciplinary courses related to key qualifications are divided into three sub-areas:

Overarching reference: Embedding the subject of study

Students are enabled to embed their subject of study in social, historical, legal or professional contexts (depending on the focus of the course). They are able to recognize, analyze and evaluate overarching subject-related connections and their significance. The students gain an insight into the networking possibilities of the subject and application possibilities of their field of study in professional life.

Scientific cultures

Students become familiar with the theories and methods of other scientific cultures, learn to deal and work interdisciplinarily with students from other fields of study, can discuss and evaluate current controversies from individual disciplines, recognize the importance of cultural framework conditions for different scientific understandings and applications, know gender-related perspectives on different subject areas and the effects of gender differences, and can deal intensively with application examples from foreign disciplines.

Action-oriented courses

Students are enabled to apply theoretical knowledge in an action-oriented manner. They acquire procedural knowledge (knowledge of procedures and courses of action, application criteria for certain procedures and courses of action) as well as metacognitive knowledge (including knowledge of their own strengths and weaknesses).

Depending on the focus of the course, students acquire the ability to

- impart knowledge and apply communication techniques,
- conduct discussions and negotiations effectively, reflect on themselves and evaluate themselves appropriately,
- work cooperatively in a team, manage conflicts,
- lead teams,
- use information and communication media or
- express themselves in another language.

The action-oriented courses enable students to use knowledge acquired in other areas more effectively, to work more easily and constructively with other people and thus to facilitate the acquisition and development of new knowledge. They acquire key qualifications that facilitate their entry into professional life and contribute to success in all professional situations.

Master thesis

Master's Thesis in AIMS

Students are able to work independently on a scientific question from a sub-field of "Artificial Intelligence for Molecular Sciences" within a specified period of time and to present their research results adequately in written form. They are familiar with the relevant conventions of their field of research and have an insight into current topics of research.

Appendix 4 - Overview of Modules Including Study Achievements, Examinations and Credit points

Abbreviations:

LP - credit point(s
PL - Examination Achievement
SL - Study Achievement
Kl. - Written Exam (APO §9a)
Kl.+ - Written Exam+ (APO §9j)
MP - Oral Exam (APO §9b)
MP+ - Oral Exam+ (APO §9k)
Presentation - Presentation (APO §9f) incl. Written Elaboration
CompProg - Creation and Documentation of a Computer or Software Program (APO, §9g)
StA - Student Research Project incl. Written Elaboration and Presentation (APO §9l)
ÜbA - Completion of Exercises or Homework (§ 5, number b)
Protocol - Protocol (§5, point c)
LabJ - Laboratory Journal (§5, number d)
expA - Experimental Work (APO §9h)
expA inkl. Koll. - Experimental Work incl. Colloquia (§ 5, point a)

(AP) In the modules marked with (AP), mandatory attendance is required in the associated lab courses and lab course preparation seminars (see § 7 para. 2).

Basic Area (Compulsory Modules)

Module	Study achievements	Examinations	LP
AM-P-1 Introduction to AIMS	Presentation		5
AM-P-2 Mathematics for Engineers A		Kl. (180 Min)	8
AM-P-3 Programming in Python and Python Lab (AP)	CompProg		8
AM-P-4 Scientific Software Engineering – Lab (AP)	ÜbA	Kl. (120 Min) or MP (30 Min)	5

Advanced Area (Compulsory Elective Area)

Module	Study achievements	Examinations	LP
AM-V-1 Introduction to Machine Learning		Kl. (90 Min) or MP (30 Min)	5
AM-V-2 Pattern Recognition		Kl. (90 Min) or MP (30 Min)	5
AM-V-3 Computer Lab Pattern Recognition (AP)		CompProg	5
AM-V-4 Deep Learning Lab (AP)	ÜbA Presentation		5
AM-V-5 Methods of Uncertainty Analysis and Quantification		Kl. (90 Min) or MP (30 Min)	5

Profile Area A "Chemical Synthesis and Drug Design" (Compulsory Elective Area)

Module	Study achievements	Examinations	LP
AM-A-1 Reaction Mechanisms		Kl. or MP	4
AM-A-2 Organometallic Chemistry		Kl. or MP	4

Module	Study achievements	Examinations	LP
AM-A-3 Catalysis (AP)		expA (25%) Kl. or MP (75%)	8
AM-A-4 Advanced Inorganic Chemistry(AP)		Referat (25%) Kl. or MP (75%)	8
AM-A-5 Organic Synthesis Planning		Kl. or MP	4
AM-A-6 Enzyme Engineering (AP)	expA	Kl. or MP	10
AM-A-7 Fundamentals of Protein Structure Analysis (AP)	expA Referat	Kl. (200 Min.)	10
AM-A-8 Biomolecular Modelling (AP)	expA (graded)	Kl.+ or MP+ (Consideration of SL with 30 %)	8
AM-A-9 Advanced Theoretical Chemistry (AP)	ÜbA (ungraded) expA (graded)	Kl.+ oder MP+ (Consideration of SL ÜbA with 20 %; SL expA. with 20 %)	8
AM-A-10 Machine Learning in Computational Chemistry (AP)	ÜbA (ungraded) expA (graded)	Kl.+ oder MP+ (Consideration of SL ÜbA with 20 %; SL expA. with 20 %)	8
AM-A-RP Forschungspraktikum „Chemical Synthesis and Drug Design“		StA	13 - 17[a]

[a] The number of credit points to be earned depends on the scope and duration of the research internship.

Profile Area B “Spectroscopy and Imaging” (Compulsory Elective Area)

Module	Study achievements	Examinations	LP
AM-B-1 Molecular Spectroscopy	ÜbA	Kl. or MP	5
AM-B-2 Biophysical Chemistry	ÜbA	Kl. or MP	8
AM-B-3 Modern Optical Methods und Imaging		Kl. or MP	8
AM-B-4 Solar and Chemical Energy Conversion (AP)	expA inkl. Koll.	Kl. (90 Min) or MP (30 Min)	8
AM-B-5 Physical Biology of the Cell (AP)	expA	Presentation	10
AM-B-6 Sophisticated Imaging (AP)	expA	Presentation	10
AM-B-7 Chemometrics	Protokoll	MP (30 Min)	6
AM-B-8 Theoretical Spectroscopy (AP)	ÜbA (unbenotet) expA (benotet)	Kl.+ or MP+ (Consideration of SL ÜbA with 20 %; SL expA. with 20 %)	8
AM-A-10 Machine Learning in Computational Chemistry (see above)			
AM-B-RP Forschungspraktikum „Spectroscopy and Imaging“		StA	12 - 16[a]

[a] The number of credit points to be earned depends on the scope and duration of the research internship.

Profile Area C "Data-Driven Biology" (Compulsory Elective Area)

Module	Study achievements	Examination achievements	LP
AM-C-1 Molecular Microbial Evolution and Diversity (AP)	expA Kl. (90 Min.)	Kl. (120 Min.)	10
AM-C-2 Immunometabolism (AP)	expA	Presentation	10
AM-C-3 Comparable Quantitative Measurements and Metabolomics Biomarker Signature to Predict Case and Control (AP)	expA	Kl. (120 Min)	7
AM-C-4 Network Biology	ÜbA	Kl. oder MP	5
AM-C-5 Molecular Phylogenetics and Taxonomy (AP)	ÜbA expA inkl. LabJ Presentation	Kl. (120 Min)	10
AM-C-6 Data Literacy and Genome Research (AP)	expA Presentation	Kl. (200 Min)	10
AM-C-7 Applied Plant Transcriptomics (AP)	expA Presentation	Kl. (200 Min)	10
AM-C-8 Functional Genomics in Infection Biology (AP)	expA Presentation	Presentation	10
AM-C-9 Microbial Proteomics (AP)	expA Presentation	Presentation	10
AM-C-RP Forschungspraktikum „Data-Driven Biology"		StA	12 - 17[a]

[a] The number of credit points to be earned depends on the scope and duration of the research internship.

Master thesis

Module	Study achievements	Examination achievements	LP
AM-M Master's Thesis in AIMS		See APO §14 and BPO §8	30

Key qualification area

In the key qualification area, the following achievements must be completed (12 CP in total)
(**P** = compulsory / **W** = elective):

Course	Study achievements	LP	P/W
AM-KQ-1 Module "Ethics and Epistemology"	Protokoll (SL) Kl. (SL, 120 Min)	5	**P**
AM-KQ-2 Professionalization module			
Language competence [a]	Kl. oder MP	up to 7	**W**
Career guidance, work placements [b]		up to 4	**W**
Acquisition of social skills, tutoring [b]		up to 4	**W**
Interdisciplinary courses from the special lists "Ziele für Nachhaltige Entwicklung", „Pool" oder „Gender Lehrverzeichnis"[c]	[d]	up to 7	**W**

[a] Language Center courses may be taken at the following level or higher:
- Language courses in the second and third foreign language at school at least at level A2.
- German language courses may only be taken by foreign students from level B1 after prior application to be submitted to the Examination Committee.
Language courses in the mother tongue or in the official languages of the home country and English courses are not recognized.

[b] Recognition requires the submission of proof and a report reflecting on the interdisciplinary skills acquired.

[c] Further credit points can be earned in courses that serve to acquire key qualifications.

These are to be selected from the overall program (pool model) of interdisciplinary courses at the Technische Universität Braunschweig.

The Examination Committee may exclude courses from the special lists "Ziele für Nachhaltige Entwicklung“, „Pool“ or „Gender Lehrverzeichnis“ or authorise other courses. A written application must be submitted to the Examination Board for the recognition of other courses/modules for the key qualification area.

[d] Proof of performance is required for the selected courses/modules. A certificate of attendance is not sufficient. The examination modalities vary depending on the selected courses.