Master’s thesis proposals

Department of Chemistry

Academic year 2016-2017

This document contains master’s thesis proposals for the following programmes of study:

Master in Chemistry (MSCHEM)
All specializations

Master in Environmental Toxicology and Chemistry (MSENVITOX)
Specialization: Environmental Chemistry

Master in Chemical Engineering and Biotechnology (MTKJ and MIKJ)
Main profile: Chemistry

Natural Science with Teacher Education (MLREAL)
Main subject: Chemistry

Please contact the supervisor directly if you have any questions related to the proposed projects.
Chemometrics and Chemoinformatics
Applications to new materials for organic solar cells

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Master project suggestions. The master projects done in our group will be linked to ongoing research in the field of organic solar cells. There is a need to develop methods for cheaper and more efficient development of photovoltaic materials, in particular organic solar cell materials. We use a fragment-based evolutionary de novo design approach to propose new compounds with improved photovoltaic properties. In particular we study dye molecules in dye-sensitized solar cells (DSSC).

1. **de novo** design of new solar cell dyes with optimal properties using principal properties. A drawback with evolutionary de novo methods is that they require a large amount of computer resources. Another, approach is to employ principal properties (PP) in combination with experimental design. Each fragment is described by a set of scores which have been derived from a principal component decomposition of a matrix containing multiple fragments with variables describing their molecular structure.

2. **Building quantitative structure-property relationships (QSPR) models of solar cell dyes using Atoms in Molecules (AIM) electronic descriptors.** Forming predictive QSPR models for solar cell dyes requires descriptors that effectively capture the 3D electronic structure of molecules. Here descriptors based on bond critical points (BCPs) of the 3D electron density of molecules (from atoms in molecules (AIM) theory) will be investigated.

3. **Conformation dependent QSPR descriptors.** Many 3D structure descriptors are based on the geometry of the most stable conformation of a molecule. However, multiple conformations are important to understanding the properties of a molecule. Here, different approaches for incorporating conformational change in 3D descriptors is investigated.
The projects offered here will be in close cooperation with Prof. Signe Kjelstrup and with application to other projects in the group when possible.

1. **Coupled transport of heat and mass in transient states.** Most transport processes are not in steady states because the forces that drive the process are not constant in time. The variation can be cyclic, such as processes caused by the Earth’s rotation, or sudden, such as processes caused by explosions. Such situations are transient. The field of non-equilibrium thermodynamics has been well developed for steady state, but not so for transient states. This project aims to study the coupling between heat and mass transport (the Soret effect) during the transient period between equilibrium and steady state when a binary liquid mixture, initially at equilibrium, suddenly is perturbed by a strong temperature gradient. The study will be based on non-equilibrium molecular dynamics simulations and thermodynamic theory.

2. **Phase diagram for the Lennard Jones/spline system.** The Lennard-Jones/spline system is a mathematical model for simple atomic systems (the noble gases). The phase diagram for this model is only partially known. This project aims to determine the equation of state and map the phase diagram for the pure fluid and some binary mixtures. The study will be based on equilibrium molecular dynamics simulations of two-phase systems and thermodynamic theory.

3. **Determination of thermodynamic equilibrium quantities by non-equilibrium molecular dynamics.** Non-equilibrium molecular dynamics simulations provide an efficient way to determine thermodynamic properties at constant pressure (such as the heat capacity CP). In this project, we will evaluate different computational schemes for the computation of properties for liquids and gases and. In particular, we will compare the efficiency of the Small Systems Method (see project 3 by Professor Signe Kjelstrup) and non-equilibrium simulations.

**Figure 1.** A pressure wave caused by an explosion at the position $x^* = 0$ at time zero. The four curves were computed by non-equilibrium molecular dynamics and show the pressure profiles at later times when they travel with the speed of sound through the liquid.
Quantum Chemistry
Development and application of electronic-structure methodologies

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Project suggestions

Most of these projects can be adjusted to fit to a 15, 30 or 60 ECTS credit assignment.
Project 1 is suitable for a student who is interested in exploring the quantum chemical nature of molecular without doing theoretical developments, while projects 2-4 are suitable for students who are interested in theoretical developments and/or computer programming.

1. Calculations of molecular properties
   Molecular properties such as geometries, excitation energies, responses to magnetic and electric fields etc. can be accurately determined using quantum chemical methods. In this project, existing methods will be used to explore the properties of a molecule of interest.

2. Multi-level coupled cluster theory development
   Coupled-cluster theory is a highly successful hierarchy of wave function models to accurately describe molecular systems. However, its computational cost limits its use to rather small systems. The multi-level coupled-cluster model, developed at NTNU, exploits the locality of electronic properties to make coupled-cluster calculations more efficient. In this project, you will participate in current theoretical developments in multi-level coupled cluster.

3. Extending the applicability range of Hartree-Fock theory
   Hartree-Fock theory is the cornerstone for accurate ab-initio electronic-structure theories, and in itself Hartree-Fock gives a decent approximation to energies and molecular properties for molecular systems dominated by a single electronic configuration. The Hartree-Fock wave function can be applied to relatively large systems, but it is of interest to extend the applicability range even further, so that it may be applied to e.g., molecules in solutions or for active sites of enzymes.

4. Hartree-Fock theory in a non-orthogonal molecular orbital basis
   In developments of low-scaling correlated wave function models, most methods relies on the spatial locality of the molecular orbitals employed. Spatial locality of orbitals is improved when relaxing the orthogonality constraint and it is therefore of interest to develop a non-orthogonal Hartree-Fock framework, to explore the possibilities offered by the non-orthogonality of the orbitals.

5. Other applications or theoretical developments projects may also be created. Send an email or come talk to us.
Applied Theoretical Chemistry
Molecular Modeling

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Project suggestions

These projects can be adjusted to fit to a 30 or 60 ECTS credit assignment

1. Electrical insulation in liquids

We have a long-term collaboration with SINTEF Energy and ABB in Sweden to understand processes related to electrical breakdown in liquids. A project would normally involve quantum chemical calculations of ionization and electron attachment processes in high electric fields. At the moment, we are very interested in calculating cross-sections (i.e. probabilities) for processes related to electron-molecule collisions and photoionization.

2. Metal particle - molecule interactions

In several research fields it is of high interest to accurately model the interactions between molecules and metal particles, and for this purpose we use density-functional theory (DFT) calculations. In collaboration with the Catalysis group at NTNU, we study e.g. Pt and Co clusters on carbon support materials and how the interactions with the carbon material affect the catalytic activity of the metal atoms. In addition, we study molecule-coated nanoparticles, e.g. gold particles, which are important for applications in optics (with Fernando Bresme, Imperial College London).

3. Classical polarization models

We work on establishing “classical” models for electronic polarization and electron transport based on classical electromagnetism and concepts from force fields and to relate them to quantum mechanical models. This type of projects is more “theory-oriented” and may involve both mathematical derivations as well as software development in addition to calculations. Properties that we are currently interested in includes optical rotation, frequency-dependent dielectric constants and conductivity.
Non-Equilibrium Thermodynamics
Applications in renewable energy technology and nanotechnology.

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Master project suggestions. The master projects done in our group will often be linked to ongoing research projects (PhD projects). They are written in English. The projects can be experimental (proposal 2) or computational, depending on the interest (please discuss with me). Computational projects are frequently molecular simulations (see proposal 3), but also process simulations are relevant (proposal 1). Smaller or larger parts of the project can be done abroad (Spain, Germany, The Netherlands, England). The list should be regarded as examples.

1. **Nature-inspired chemical process design.** We study the entropy production in the nose of various animals in the arctic and test the hypothesis that nose has evolved to keep as much of the body heat and water as possible. What could be the bearing of this on the design of heat recuperator in a house?

2. **Thermoelectric energy conversion.** We study the ability of systems of ion exchange membranes and salt solutions, to better see how the system can exploit waste heat for power generation. Transport properties need be measured for this purpose. The performance of the generator can then be modelled.

3. **Simulations of thermodynamic data and transport properties for thin film technologies.** We have invented a new way to find properties of small systems, knowing the behavior in the ordinary bulk. This may allow us to study properties of small systems, for instance the thermodynamic factor $\Gamma$ (right) for CO$_2$ adsorbed on graphite (left).
Molecular Modeling
Development of Advanced Simulation Techniques

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Project suggestions

In our group there are several possibilities for master projects. We welcome students from many study directions. Depending on personal interest, a master-thesis project can be pure theoretical (pen-and-paper mathematics), involve programming, or simply use existing software for running simulations and analyzing data. Contrary to what students often believe, one does not have to be a mathematical genius to perform a research project within theoretical chemistry. It is possible to go into depth regarding theory or software development if you want, but a lot of exciting research is done by applying existing programs in a similar way as an experimentalist uses an instrument. An interdisciplinary master-project is possible since we are dealing with many types of challenges, which could be tackled by chemists, mathematicians, computer scientists, chemical engineers, nanotechnology students, biotechnologists, or physicists. Here we list possible projects, though these are a few of the possible projects and if you have an own idea, I am happy to discuss it with you!

1. **QuanTIS: a new way to combine classical dynamics and quantum-mechanics.**
   In this master project you will contribute to our main research activity which implies a completely new way to combine classical molecular dynamics and quantum mechanics (See e.g. Nobelprize chemistry 2013). The revolutionary new aspect that we are developing is that we connect these methods in the time domain not just in space. The method would allow us to study enzymatic and complex catalytic reactions involving large systems, long time-scales at quantum mechanical accuracy.

2. **Coalescence and film rupture.** In this project reaction path sampling will be applied to study the film rapture between bubbles present in liquid emulsions, which is a key phenomena in coalescence process. The selected case of study consist in oil-water emulsions, which is a relevant system for oil industry.

3. **Understanding DNA Dynamics.** For decades, experimental and theoretical scientists have been fascinated by the thermal DNA denaturation. It is biologically relevant since the opening of the double helix in an important step for the transcription of the genetic code. We have tested and developed simplified models to simulate the movements of DNA. In addition we developed special algorithms to run simulations much faster than was possible before. This allows us now to get a better idea on how the rate of denaturation changes with respect to the sequence and other factors. In addition, it allows us to test and compare results with experiments and to improve present models with this information.

4. **MORE INFO ON THE WEBSITE: www.van-erp.org/**
Project suggestions

1. **Improvement the analytical methods for iron determination in seawater**

Iron is an essential micronutrient for microbial organisms (bacteria and phytoplankton) in oceans. Iron is a limiting nutrient in almost 40% of the Ocean, especially in the Antarctic waters and most of the Southern Ocean. It is one of the key element which has important role for regulation of the atmospheric CO2 hence Climate of the Earth.

Determination of iron and its forms in seawater is a challenging task. The student will test various factors to improve the determination of the iron by using Sea-FAS pre-concentration instrument and High Resolution Inductively Coupled Plasma - Mass Spectrometry (HR-ICP-MS).

2. **Impact of CO2 seepage from subsea-bed CO2 storage sites on the biogeochemistry of trace elements at the sediment–water interface**

This project will be part of two projects (an EEA project and a NFR projects with international partners). The task is to follow the mobilization of the different trace elements (both toxic and bio-essential elements) mobility and distribution of the surface sediment. Multi analytical techniques will be used to determine the distribution and transformation of elements (i.e. Sea-fast pre-concentration technique, ICP-MS, sediment sequential extraction etc).

3. **Impact of CO2 seepage from subsea-bed CO2 storage sites on the biogeochemistry of dissolved organic matter (DOM)–metabolites at the sediment–water interface**

This project will be part of two projects (an EEA project and a NFR projects with international partners). The task is to follow the mobilization and characterization of the organic matter, their mobility and distribution at the sediment- water interface. Multi analytical techniques will be used to determine the distribution and transformation of DOM (i.e. Synapt G2-S Q-TOF and Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS))
**Environmental Chemistry**

**Marine Organic Environmental Chemistry**

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**Project suggestions (can be adjusted to both 60 and 30 credits)**

1. **Oil spill forensics – Mapping sources for illegal oil spills**
   SINTEF is the national laboratory for oil spill identification in Norway. MSc projects are available focusing either on available data from the established database at SINTEF for fingerprinting and identification of possible sources for illegal oil spills. The information from an oil spill sample (gas chromatography and mass-spectrometry) is compared with the database by using both univariate statistics (t-test) and more sophisticated multivariate statistics. One focus on such a project could be to utilize more of the analytical data generated and study how oil weathering processes (e.g. evaporation, biodegradation and photo-oxidation) influence oil spill identification by using modern multivariate statistical methods. A large dataset of stranded oil spills are available from earlier KJ3050 field surveys along the coastline outside Trondheim. Also this year KJ3050 will perform a survey for new samples. These samples can be analyzed to determine the sources for these oil spills (offshore installations in the North Sea, coastal traffic (ships) or even foreign sources) Students could do their own analysis on new or stored oil samples or work on already generated data from earlier oil spills.

2. **Fate of subsurface releases of oil (blow-outs) as a function of release conditions and oil types**
   The Macondo oil spill in the Mexico gulf in 2010 created new interest and focus on this special type of oil spills. This has been an important research field at SINTEF for the last twenty years. We perform both theoretical and experimental analytical projects regarding the physics, fate and modeling of subsurface oil releases. We have both basin and bench-scale experimental facilities we use in our projects. We study droplets size distributions of the released oil as a function of release conditions, oil chemistry and injection of surface active components (dispersants). Students can work on already generated data, participate in ongoing industry project at SINTEF or generate their own data with our bench-scale apparatus.

3. **Weathering processes in marine oil spills**
   When oil is released or spilt in the marine environment many weathering processes will alter the chemical and physical properties of the oil as a function of time (emulsification, evaporation, photo-oxidation, natural dispersion etc.). Knowledge regarding how changes in these properties influence the properties of the oil spill is important for both understanding environmental damage and choice and effect of oil spill contingency methods.

Other MSc projects related to marine organic pollutants, initiated by students, could also be of interest. Do not hesitate to make contact for further discussions!
Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment.

1. Study of kinetics of organic reactions in a microwave-assisted flow-chemistry micro-reactor.

2. Analysis of organic contaminants in environmental samples.
Environmental and Analytical Chemistry

Fields of research: The roles of trace elements in the environment and in human health

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Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment

1. Mapping the contents of trace elements in foodstuffs, drinking water, etc. Our research group's HR-ICP-MS instrument is the most powerful analytical technique currently available for multielement analysis at low concentrations. Thus, we can provide data for trace elements for which there is little data in the literature. Examples of recent master projects in this area are mapping of trace elements in tea, in drinking water in Nord-Trøndelag county, in trace element/vitamin supplements, and in baby food. Any suggestions from the student is welcome.

2. At our department, we have a large collection of samples of vegetation, soil and other material representing the whole country or specific geographical regions. These samples were collected to gain knowledge of both the natural distribution of trace elements and the influence of regional and local pollution. However, at the time of collection we did not have access to the high-quality analytical instruments that we now have, so it would be very interesting to analyse these valuable samples using ICP-MS. Master projects using some of this material could be supplemented by collecting additional samples in the field (e.g. to investigate possible time trends).
Project suggestions

Most of these projects can be adjusted to fit a 30 or 60 ECTS credit assignment.

Master projects within;

- developing analytical methods and routines for industry and environmental monitoring.

Please contact me for detailed projects (e.g. specific projects connected to the aquaculture industry, metallurgical industry etc.)
Structural chemistry
Application of synchrotron techniques in material science and nanotechnology

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The research group consists of one post doc, two PhD’s and currently 6 master students. A master project typically involves synthesis and functionalisation of new materials, such as metal containing aerogels or zeotypes. You will be trained in a range of characterization techniques such as XRD, BET, SEM, FTIR, all crucial for understanding the material. We travel frequently to synchrotrons like the ESRF in Grenoble to do x-ray absorption spectroscopy (XAS) to further study our materials at the Swiss Norwegian Beamline (SNBL). We have collaborations with University of Glasgow UK and Newcastle Australia.

Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment.

1. Co-introduction of Co and Mo into mesoporous SBA-15 for the ammonia synthesis
2. Developing a synthesis route for functionalisation of silica aerogels with Re

   *Our ongoing collaboration with University of Glasgow investigating the effect of Re and Mo on cobalt-supported materials for the ammonia synthesis.*

3. Functionalisation of Fe into silica aerogels; structural effect of metal loading

   *The goal is to develop single-site iron in hydrophobic aerogels which are interesting for a range of catalytic application.*

4. Characterisation of hierarchical SAPO-34; are micro and mesopes available
5. Investigating the effect of porosity Cu-zeotypes for the reduction of NOx

   *We are currently trying to make porous materials with super-highways for gas reactants travelling to micro reactors inside the material.*
Environmental and analytical chemistry

For information on other research fields in the environmental and analytical chemistry group, contact:

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Environmental chemistry

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Cultural Heritage
Project suggestions

Most of these projects can be adjusted to fit to a 30 or 60 ECTS credit assignment

1. **Organic molecules for new solar cells**

   Solar cells based on organic molecules have the prospect of being cheaper and allowing for other applications than currently employed silicon based technology. The group has therefore started research into design of new molecules for organic based solar cells. The work will be done in collaboration with Associate Professor Odd Reidar Gautun, Professor Bjørn Alsberg and Professor Svein Sunde.

2. **Kinase inhibitors for treatment of cancer and neurodegenerative diseases.**

   The group is developing new kinase inhibitors for cancer treatment and neurodegenerative diseases. Master projects will involve development of synthetic methodology and the preparation of new potential inhibitors. Molecular modelling is employed to plan the projects and to aid understanding of structure-activity relationships. The candidate compounds are characterised by enzymatic and cellular assays in other research groups or by contract research organisations.
Biocatalysis in organic chemistry
Synthesis of enantiopure bioactive molecules by use of biocatalysts

Project suggestions

1. **Synthesis of enantiomerically pure (S)-atenolol** ((S)-2) from (R)-2-(4-(3-Chloro-2-hydroxypropoxy)phenyl)acetamide, (R)-1, (99 % ee), Scheme 1. A method for synthesis of (R)-1 has been developed (Scheme 2), and this synthesis will be the first step in the master work. I.T. Lund, P.L Bøckmann, E.E.Jacobsen, Tetrahedron 2016, (30 ECTS).

![Scheme 1](image1)

![Scheme 2](image2)

2. **Synthesis of enantiopure β-blockers and other bioactive molecules by use of enzymes.** Many pharmaceutical active ingredients (API) in drugs are secondary amino alcohols. Many of them are manufactured both with the racemic and the enantiopure API, however, pure enantiomers are preferred (Chiral Switch, FDA 1992). Development of enzyme catalysed methods for synthesis of pure enantiomers involves synthesis of racemic compounds, kinetic and mechanistic studies of enzyme action, analyses of enantiomers on chiral GLC and HPLC-columns, use of enantiopure building blocks in final drug synthesis. (30 or 60 ECTS). Alprenolol, pindolol (figure 1) and metaproterenol are interesting targets.

![Figure 1](image3)

Figure 1. Alprenolol and pindolol.
Synthetic Organic chemistry
Gold(I) catalysis in organic synthetic chemistry  (https://www.ntnu.edu/gold)

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co-supervisor: PhD stud. Melanie Siah

Master Projects
The main objectives of the project are:
- develop new selective gold catalysed cyclization reactions.
- incl. mechanistic studies (e.g. isotope labelling, NMR spectroscopy)
- elucidate structure of novel compounds.

Projects (30/60 ECTS credits) on current research topics in the group will be defined by contact with prof. Anne Fiksdahl

Background gold catalysis in the Fiksdahl group
Gold(I) catalysis of organic reactions has become a rapidly expanding field in recent years after being neglected by organic chemists for a long time. Gold(I) catalysts react in very selective ways and may give access to highly complex molecules and challenging new structures. Alkynes are successfully used as substrates for gold catalysis.

The Fiksdahl group is working with advanced metal-organic catalysis in organic synthesis. We have shown that specific highly reactive and versatile substrates are able to follow a diverse range of novel Au(I)-catalysed chemoselective pathways, as shown by published results from current and previous master / PhD projects in the group. The novel approaches readily allow preparation of a great variety of new complex poly-functionalised products:

![Diagram of NOVEL CYCLOADDITION REACTIONS]
Synthetic Organic chemistry
Synthesis of novel absorbents with optimal CO₂ capturing properties

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Co-supervisor: PhD stud. Sigvart Evjen

Master Project
The main objectives of the project are:
- synthesize new promising absorbents (amines, imidazoles, ionic liquids/ILs) for CO₂ capture, based on theoretical calculations;
- characterize and test newly synthesized absorbent candidates (thermodynamic and solvation properties)

in order to obtain adsorbents with optimal reactivity toward CO₂, and greatly reduced absorbent regeneration energy, without sacrificing environmental friendliness and operational stability. The project will involve classical organic synthetic chemistry (incl. purification, characterization; flash chrom. recryst., dest, ion exchange, NMR, IR, HRMS).

Projects (30/60 ECTS credits) will be defined by contact with prof. Anne Fiksdahl.

Background CO₂ capture:
Capturing CO₂ using absorption with amine solutions has been used industrially for years:

a) Organic amines (prim/ sec/ tert) being used for CO₂ capture:

b) Structures of ILS:

In order to meet the goals for global reduction of CO₂, an improvement of current technologies for carbon dioxide capture and storage (CCS) is needed. Hence, the efficiency of new methods and their suitability for large-scale industrial applications must be increased.
- The present project is applying de novo design to develop improved new absorbents.
- The most promising candidates for CO₂ capture absorbents is prepared by org. synthesis.
- A microscale measurement equipment is built at SINTEF Matr. and Chem. as part of the project in order to enable experimental testing of small amounts of synthesized absorbent.
- Accurate measurements of the most important thermodynamic properties give information on the CO₂ absorption capacity.

The present project is aiming at increasing the efficiency of amine-based capture technology to be applied in the development of the next generation of absorbents, such as new amines, imidazoles and ionic liquids (ILs, see b) above).

The Fiksdahl group is responsible for the organic synthesis and testing part of the project.
Project suggestions for 2016

1. Synthesis of the novel anti-inflammatory compound

In a recent bioactivity guided study of plant Sclerochloa dura, carried out at the Departments of Biology and Chemistry, NTNU, a new, potent anti-inflammatory compound has been identified (Fig. 1). In order to continue its further investigation as a lead compound, a new project has been launched with the aim of synthesizing the new compound (Scheme 1).

Figure 1. New anti-inflammatory compound

The goals of a master project are:
1) to optimize selected reactions from the proposed synthetic route;
2) to scale up the reactions to a 10g-scale.

**There is place for 2 master students on this project.**
The master project will be co-supervised by Assoc. Prof. Bård Helge Hoff.

2. Isolation and structure elucidation of natural bioactive molecules from *Herniaria incana*

We have recently started a study aimed at a close investigation of saponins and flavonoids from *H. incana*, a species belonging to Herniaria genus. So far we have isolated and identified saponin 2 (Fig. 2).

The goal of this master project is to proceed with further separation of the earlier obtained fractions, by using various chromatographic techniques, and isolation of pure compounds. Identification of the isolated compounds will be done by various 1D and 2D NMR experiments and MS analysis.

**There is place for 1 master student on this project.**

Figure 2. The saponin isolated from *H. incana*
Synthetic organic chemistry
Methodology and total synthesis

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Master projects 2016 (realfag / siv.ing.)


![Example of a target structure](image)

2. Topic: Synthesis of novel antibiotics inspired by marine natural products (several projects). Infectious diseases are the leading causes of death worldwide and account for more than 13 million deaths annually, including nearly two-thirds of all childhood mortality at less than 5 years of age (Report on infectious diseases. Removing obstacle to healthy development. WHO, Geneva 1999). Antibiotic resistance is escalating and affects a very broad range of human diseases including tuberculosis, cholera, malaria and AIDS. These master projects will constitute subprojects of an overall project in development of new antimicrobial agents based on marine bioactive compounds. The overall project is a multi-disciplinary collaboration of specialists in organic synthesis, drug design and optimization, biochemistry, microbiology and biotechnology from the four Norwegian universities in Tromsø, Bergen, Stavanger and Trondheim (UiT, UiB, UiS and NTNU). One example of an antimicrobial compound isolated from the Barents Sea is shown below (J. Nat. Prod. 2011, 74, 837). Since this compound is highly complex, we wish to prepare libraries of simplified model compounds for biological testing and structure-activity relationship studies (SAR).
Synthesis of highly conjugated unsaturated amino acids

Essential amino acids are saturated compounds. The few natural or synthetic mono or diunsaturated amino acids show distinct biological properties, e.g. as antibiotics and enzyme inhibitors. Highly unsaturated conjugated amino acids have not been detected in nature and have not been synthesized.

The aim of this master project is the synthesis of a highly unsaturated conjugated amino acid (1).

An obvious first try to polyene amino acids would be the classical Strecker reaction. Treatment of a polyunsaturated aldehyde with primary amines in the presence of molecular sieves could afford the corresponding imine, which, without isolation, would react with trimethylsilylcyanide (TMSCN) to nitrile. The hydrolysis reaction -CN → –COOH is expected to be the most demanding step in the reaction to unsaturated amino acid. The rather harsh reactions conditions have certainly to be modified to keep yields acceptable.

Alternatively, a polyene aldehyde or polyene ketone is treated with KCN, ammonium acetate or ammonium carbonate affording the corresponding hydantoin, which can be hydrolysed to the amino acid (Bucherer-Berg synthesis).

Another possible synthesis route is based on a Wittig reaction starting from a commercial amino acid, which after several transformations, (protection of amino group and reduction to alcohol, will react with the Wittig salt of a carotenoid.)