

Department of Chemistry

Annual Report 2013



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Svein Jacob Kaspersen at work in the laboratory, synthesizing molecules with intended use in targeted cancer therapy. © Bård Helge Hoff

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The State of the Department of Chemistry 2013

Despite a difficult economic situation and a sudden interruption in the recruitment process from the Faculty, the department of chemistry managed to continue the positive trends started the previous years. The main focus during 2013 has been to develop research activities with external funding, and the department has managed brilliantly to develop several major projects.

The environmental and analytical chemistry group together with the Biology department at NTNU and several external partners developed a major EU financed project called OCEAN-CERTAIN. This project aims to explore the effects of climatic and non-climatic stressors on the structure and functionalities of the marine Food Web (FW) and the associated Biological Pump (BP), focusing on feedbacks and the goods and services the FW/BP delivers to the ecosystem and to human socio-economic systems, with the aim of reducing targeted uncertainties.

Similarly the applied theoretical chemistry group was granted a major project from the Research Council of Norway after an impressive A-score for an ERC consolidator project from the EU commission. This project aims to develop a method for running efficient and accurate quantum based dynamics of chemical reactions without the necessity to develop a new force field for each system which is a painful and time-consuming process.

The Research Council of Norway financed as well and through the CLIMIT program a project with the objective to establish a novel technology for efficient development of new carbon capture absorbents with optimal properties. This project was established by the applied theoretical chemistry group with close collaboration with the organic chemistry group, the department of chemical engineering at NTNU, the University of Bergen, SINTEF and the University of Notre-Dame in USA.

The European Commission allocates as well during 2013 the prestigious Marie Curie International Outgoing Fellowship for Career Development (IOF) to Professor Henrik Koch from the applied theoretical chemistry group and his project on the development of multi-level electronic correlation methods in quantum chemistry. This is a major achievement for our colleague.

2013 saw an increased focus on the quality insurance of education at NTNU, and for our department great emphasis has been put into implementation of the new system for student and course evaluations. The number of students applying to our BKJ program increases, and the number of MSc candidates is believed to increase by the start-up of our new international Master of Chemistry (MSCHEM). In 2013 NTNU invited all scientific groups at the university to propose some projects to develop and gain experience with new and innovative teaching methods. Associate professor and deputy for education at the department, Karina Mathisen, developed in close collaboration with the Material Technology department a project named "Virtuelle kjemiske rom" that is granted by the rector. This is a major accomplishment for the two departments that shows our constant concern in developing the state-of-the-art for educational matters. The project aims to introduce new innovative initiatives in general chemistry through videos and animations of chemical principles, web-based self-testing and interactive student response systems-

8 new PhD students (Nicolas Sanchez, Thomas Aleksander Bakka, Melanie Huey-San Siah, Shokouh Hagdani, Mahmoud Moqadam, Sailesh Abburu, Rolf Heilemann Myhre and Jin Han) were welcomed to the department in 2013, while 5 PhD students completed and defended their dissertations (Syed Majid Bukhari, Tina Kristiansen, Silje Melnes, Eugenia Mariana Sandru and Thor Håkon Krane Thvedt). The number of PhD students in the department at the end of 2013 counted 35. The department welcomed as well in 2013 three new post-doc: Chris Daub, Agnieszka Zlotorowicz and Tina Kristiansen.

The number of scientific papers published in international peer-reviewed journals has increased substantially compared to the previous years. In 2013, the number reached a total of 81 (data from Cristin), against 61 in 2012.

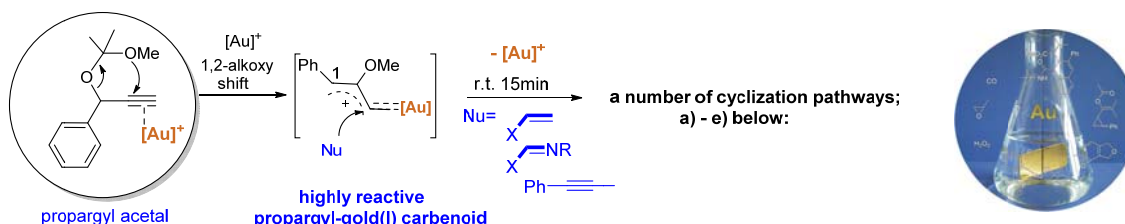
*Marie-Laure Olivier
Head of Department*



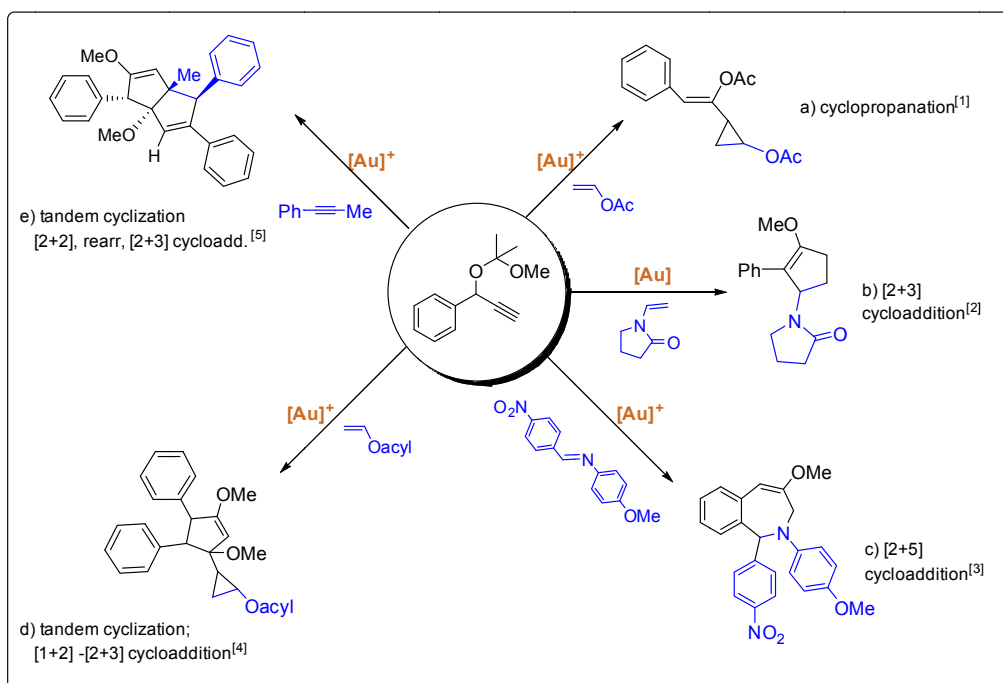
Gold catalysis; background

Gold catalysis has been neglected by organic chemists for a long time. However, homogenous gold catalysis of organic reactions has in recent 5-10 years become a rapidly expanding field. Gold(I) complexes are known to be efficient catalysts for the activation of C-C multiple bonds towards nucleophilic attack.

The Fiksdahl group (<http://www.ntnu.edu/gold>) has carried out a comparative study on chemoselective gold(I) catalysed cycloadditions of *propargyl substrates*.^[1-5] Through these investigations it has been demonstrated that propargyl acetals form *highly reactive propargyl-gold(I) carbenoid intermediates*, following different novel cyclization pathways by reaction with multiple bonds reactants:



A great variety of new cyclic products were readily prepared by the novel reactions:



Publications within Au-propargyl chemistry:

- [1] Sperger, C. A.; Tungen, J. E.; Fiksdahl, A. *Eur J. Org. Chem.* **2011**, 3719.
- [2] Iqbal, N.; Sperger, C. A.; Fiksdahl, A. *Eur J. Org. Chem.* **2013**, 907.
- [3] Iqbal, N.; Fiksdahl, A. *J. Org. Chem.* **2013**, *78*, 7885.
- [4] Siah, [M. H.-S. Maya Kaur, M.; Iqbal, N.; Fiksdahl, A. *Eur J. Org. Chem.* **2014**, in press.
- [5] Siah, [M. H.-S. Hogsnes, M. C.; Iqbal, N.; Fiksdahl, A. to be published.

Correlation of lipoplex morphology and transfection efficacy for pyridinium-based cationic lipids by means of synchrotron small angle x-ray diffraction.

This is a project undertaken in collaboration between the Department of Chemistry, Norwegian University of Science & Technology and the Department of Physics, University of Stavanger; Premedical Unit, Weill-Cornell Medical College – Qatar; Department of Chemistry, University of Victoria, Canada and the Faculté de Pharmacie, Université Paris Sud XI.

Introduction

While promising, cationic lipid-mediated gene delivery can still benefit from improvements in lipid design and lipid-DNA (lipoplex) formulation. The putative mechanism of cellular lipoplex uptake is believed to occur by endocytosis, where the key

influential factors are lipoplex size and morphology; lamellar and inverted hexagonal (Fig. 1). Ideally, the initial lipoplex packaging would have the lamellar phase upon uptake, followed by a phase transition to hexagonal, facilitating cargo release into the cytosol. The cationic lipid structure defines its molecular packing parameter, S , which in turn controls the lipid phase transition. An attempt was made to correlate a molar weighted average packing parameter (S_{mix}) for the overall cationic and neutral co-lipid mixture within a lipoplex formulation with the anticipated lamellar ($S < 1$) or hexagonal ($S > 1$) lipoplex morphology.

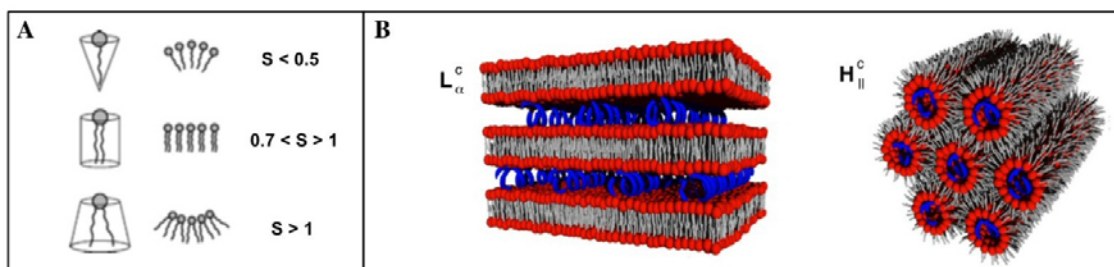


Fig. 1. Schematic representations of (A) the phase structure of cationic lipids as a function of their packing parameter, S (adapted from: Wasungu L, Hoekstra D. J. Control. Release 2006, 116, 255-264), and (B) of the phases of lipid-DNA complexes: complexed lamellar (left), and complexed inverted hexagonal (right). (from: Tresset BMC Biophysics 2009 2:3).

Objective

To test the influence that cationic lipid shape (defined by Eqn. 1) has on the molar weighted average packing parameter, S_{mix} , for the overall cationic and neutral co-lipid mixture, and how this influences the lamellar / hexagonal phase structure of pyridinium-lipid/DNA complexes (lipoplexes) using small-angle x-ray diffraction (SAXRD), and

ultimately correlating lipid shape with transfection efficiency.

$$\text{(Eqn. 1)} \quad S = V_C / (a_0 \times l_c)$$

Where V_C is the volume of the lipophilic tail of the amphiphile, a_0 is the cross-sectional area occupied by the headgroup of the amphiphile, and l_c is the critical chain length.

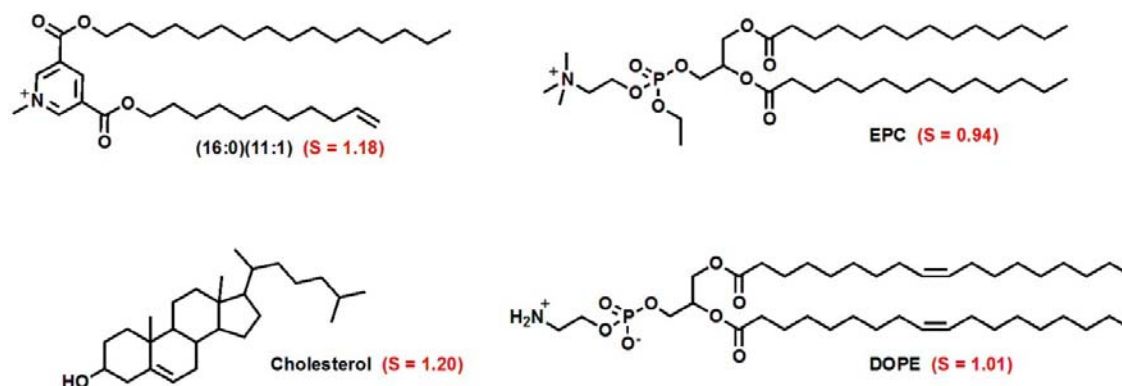


Fig. 2. Chemical structures of pyridinium lipid, (16:0)(11:1), commercial control, EPC, and neutral co-lipids, cholesterol and DOPE, and their calculated shape parameters, S .

Methods

Molecular structure parameters and partition coefficients were calculated for the individual lipids within each pyridinium-lipid containing formulation using fragment additive methods, and the derived shape parameters of the component lipids (Fig. 2) were used to calculate the mole ratio weighted shape parameter of the mixture, S_{mix} (Table 2).

Liposomes were prepared from the synthetic pyridinium-based cationic lipid, (16:0)(11:1), in combination with the commercial lipid EPC and co-lipid, DOPE or cholesterol (Fig. 2). Lipoplexes were then formulated by incubating the liposomes with

plasmid DNA (pDNA) at various N/P (+/-) molar charge ratios, and subsequently characterized by gel retardation, DNase I degradation, biocompatibility and β -galactosidase (β -gal) transfection assays using Chinese Hamster Ovarian (CHO-K1) cells. Lastly, lipoplexes at N/P molar charge ratio 3 (only) were analyzed by small angle x-ray scattering SAXS(SAXRD) at the European Synchrotron Radiation Facility (ESRF), Grenoble, France, on the bending magnet, beamline BM26.

Results

Table 1. Summary of liposome and lipoplex* particle sizes and polydispersity index (Pdl) measured by dynamic light scattering for the various formulations.

Lipid molar ratios used				Particle sizes for 2mM Liposomes (Pdl)
(16:0)(11:1)	EPC	DOPE	Chol	Size in nm
0	3	1.5	-	396.0 (0.5)
0.5	2.5	1.5	-	212.9 (0.2)
1	2	1.5	-	374.8 (0.3)
1.5	1.5	1.5	-	229.5 (0.2)
2	1	1.5	-	652.8 (0.4)
2.5	0.5	1.5	-	445.9 (0.4)
0	3	-	1.5	312.5 (0.8)
0.5	2.5	-	1.5	808.0 (0.4)
1	2	-	1.5	558.5 (0.4)
1.5	1.5	-	1.5	826.4 (0.5)
2	1	-	1.5	786.0 (0.6)
2.5	0.5	-	1.5	354.1 (0.4)

* Particle sizes of all lipoplexes (N/P = 3) was >1,000 nm (with Pdl ranging from 0.3-0.8).

Conclusions

The lamellar to hexagonal packing transition predicted by S_{mix} calculations was in agreement with that determined by SAXRD, and correlated with the highest level of transfection (at N/P = 3) for the lipid-DNA lipoplexes composed of the (16:0)(11:1)/EPC when DOPE was employed as co-lipid. The same was not observed when cholesterol was the co-lipid.

Acknowledgments

This work was made possible in part by a grant from the Qatar National Research Fund under the National Priorities Research Program, award NPRP08-705-3-144. Its contents are solely the

responsibility of the authors and do not necessarily represent the official views of the Qatar National Research Fund. Beamtime on the Dutch-Belgian beamline BM26 was provided in collaboration with the Swiss-Norwegian beamline at the ESRF, Grenoble, France. The authors wish to thank G. Portale and D.H. Merino for technical assistance in setting up the SAXRD measurements. Funding from the National Science and Engineering Research Council of Canada is gratefully acknowledged.

David G. Nicholson

Enantiopure dihalocyclopropyl alcohols, building blocks for insecticides

Insecticides from natural sources

The cyclopropane moiety occurs in a number of natural products with biological activity. Normally, such compounds are chiral. They may contain stereogenic centers either within the ring or outside.

The most well known among such compounds are the pyrethrins, insecticides originally isolated from a composite (now Asterae) plant known as *Pyrethrum cinerariaefolium*, now renamed as *Chrysanthemum cinerariaefolium*, Figure 1.¹

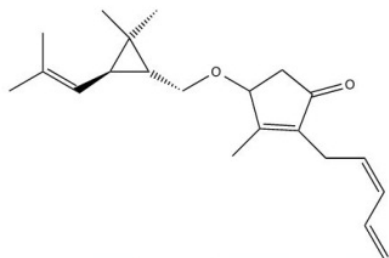


Figure 1. *Chrysanthemum cinerariaefolium* and structure of Pyrethrin-I.¹

The pyrethrins are neurotoxins that attack the nervous systems of all insects. They are biodegradable and have normally a half-life of 12 days.

Industrial production of insecticides

Today, a range of insecticides with the origin from the natural compounds are synthesised industrially.² They are known as pyrethroids and their biological activity depends on distinct stereochemistry. Hence, synthesis may be demanding.

One example is permethrin, which has four possible enantiomers, *trans*-permethrin is shown in Figure 2.

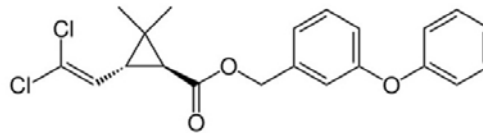


Figure 2. *trans*-Permethrin.

Enantioselective synthesis of cyclopropanes

Providing enantiomerically pure compounds may in principle be achieved by enantioselective synthesis or by resolution of a racemic mixture. Both methods have their characteristics, advantages and limitations. Enantioselective synthesis can in principle give 100% of a pure enantiomer, a racemic mixture contains both enantiomers, which have to be separated.

The most well-known way to obtain cyclopropane compounds is via the Simmons-Smith reaction. This reaction converts an alkene into a cyclopropane compound utilising CH_2I_2 and a Zn/Cu couple.³

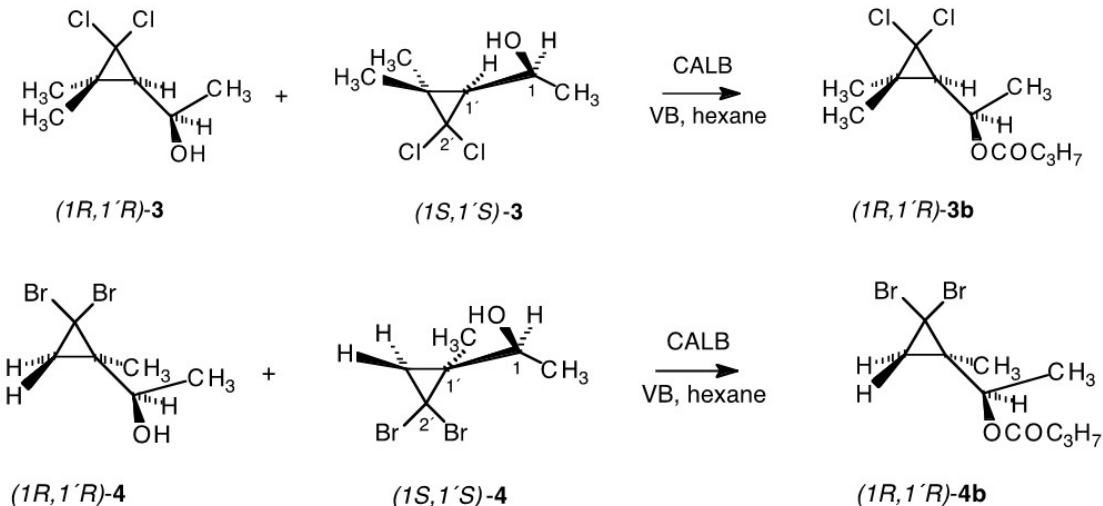
Furthermore, addition of dihalocarbenes to alkenes, affording the corresponding dihalocyclopropanes is another useful reaction. This reaction may to some extent be enantioselective, provided the substrate contains stereogenic centers.

By using kinetic resolution a product can be obtained enantiopure provided the yield is less important. Dynamic kinetic resolution, in which the substrate is racemised during the process, overcome this problem, however, it is not always feasible.

We have chosen enzyme catalysed kinetic resolution in order to obtain enantiopure cyclopropane derivatives.

The two secondary alcohols ($1R^*,1'R^*$)-**3** and ($1R^*,1'R^*$)-**4** gave excellent results with lipase B from *Candida antarctica* (CALB) and vinyl butanoate as acyl donor. (Scheme 1)⁴

The enzymatic esterification of ($1R^*,1'R^*$)-**3** was very selective and 50% conversion was reached after 7 h ($E \approx 1000$), giving the butanoic ester ($1R,1'R$)-**3b** in 99% enantiomeric excess (ee) and the remaining alcohol ($1S,1'S$)-**3** in 98 % ee.



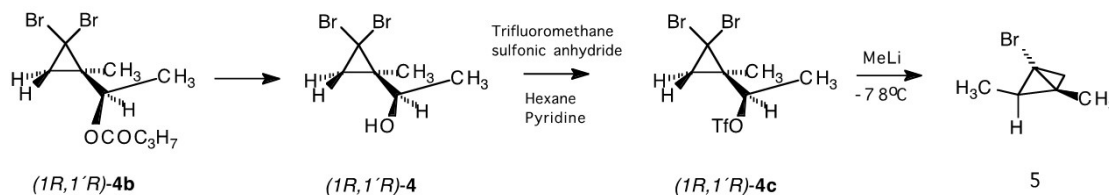
Scheme 1

An *E*-value of 1000 means that the *1R,1'R*-enantiomer reacts 1000 times faster than the *1S,1'S*-enantiomer in the esterification reaction. Similar results were obtained for esterification of the dibromo compound **4** giving (*1R,1'R*)-**4b** in 99% ee after 5 days. The pure enantiomers **3**, **4**, **3b** and **4b** were obtained in 40-60 % yield.

In addition to being building blocks for pyrethrins, enantiopure dihalocyclopropane compounds may

be starting materials for different aromatic compounds and carbocyclic compounds.

Enantiopure dihalocyclopropanes are also starting materials for the first known enantiopure bromo and chloro bicylobutanes. Cyclisations of the dihalocyclopropanes by triflate addition are in progress in our group. (Scheme 2)⁵



Scheme 2

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2. Martel, J., **1992**. The development and manufacture of pyrethroid insecticides. In: Collins, A.N., Sheldrake, G.N., Crosby, J. (Eds.), *Chirality in Industry*. John Wiley & Sons, New York.
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4. Jacobsen, E.E., el-Behairy, M.F., Skattebøl, L., Anthonen, T. Enantiopure dihalocyclopropyl alcohols and esters by lipase catalyzed kinetic resolution *J. Biotechnol.* **2013**, 168, 284-288.
5. Unpublished results

Elisabeth Jacobsen

Thorleif Anthonen

Anti-inflammatory and Antioxidant Activities of *Sclerochloa dura* (Poaceae)

Abstract: The plant *Sclerochloa dura* is traditionally used in South-East Serbia to treat menstrual disorders characterized by pain and excessive bleeding. According to subjects' statements, a reduction in bleeding and pain is experienced shortly after oral intake. The focus of this investigation was to determine the inhibitory effects of the plant on the arachidonic acid (AA) cascade along with the spectrophotometric determination of antioxidant capacity. The AA release assay was performed using the human fibroblastlike synoviocyte cell line SW982 to determine the AA release and hence phospholipase A₂ (PLA₂) activity. The crude extract and subsequent fractions of *S. dura* inhibit IL-1 induced release of AA in a time- and dose-dependent manner in SW982 cells. The IC₅₀ for the crude

extract is 1.5 mg/mL at 4 h and 24 h of stimulation. Treating the cells with 0.22, 0.11 and 0.06 mg/mL of methanolic fraction resulted in 97%, 91%, and 63% inhibition of AA-release, respectively. One milligram of the crude extract contained 34.78 µg pyrocatechol equivalent phenolic content, 22.80 µg quercetin equivalent flavonoid content and antioxidant activity of 70.11 µg α-tocopherol equivalents. Strong inhibitory effects of the *S. dura* extracts on AA cascade may explain the reported pain- and discomfort relieving effects.

Key words: Arachidonic acid release assay, Cytosolic phospholipase A₂ enzyme, Flavonoid content, Free radical scavenging activity, Phenolic content, SW 982 fibroblastlike synoviocytes.

Introduction

Eicosanoids such as prostaglandins and leukotriens are derivatives of the Ω-6 fatty acid (AA) and act as potent lipid mediators of inflammation¹. AA is released by the action of phospholipase A₂ (PLA₂) enzymes by hydrolysis of the *sn*-2 ester bond of membrane glycerophospholipids. PLA₂ enzymes are primarily sorted into five categories; secretory PLA₂ (sPLA₂), cytosolic PLA₂ (cPLA₂), Ca²⁺-independent PLA₂ (iPLA₂), platelet-activating factor acetyl hydrolases (PAF-AH) and lysosomal PLA₂s^{2,3}. Alongside the ongoing elucidation of the roles of different PLA₂ isotypes in physiology or pathophysiology of different diseases⁴, there is great interest in the development of different PLA₂ subtype-specific inhibitors to treat human diseases⁵. Pro-inflammatory cytokines, such as TNF and IL-1β, activate PLA₂ enzymes, mainly the arachidonyl specific cPLA₂-IVα isotype, resulting in the subsequent release of AA and generation of proinflammatory eicosanoids⁶⁻⁸. Also, we have previously shown that activated TNF and IL-1β may lead to increased transcription of the cyclooxygenase 2 (COX2) and cPLA₂-IVα genes, further propagating inflammation by increased availability and metabolism of AA into proinflammatory eicosanoids^{8,9}. In addition to the association to inflammation, increased availability of AA has also been associated to heavy menstrual bleeding¹⁰. Prostaglandins such as PGE₂ and PGF₂ levels have been found to be elevated in the endometrium of women with heavy menstrual bleeding compared to women with normal menses^{11,12}. Prostaglandins contribute to uterus contractions¹³ and are thought to be a major factor in primary dysmenorrhea. By targeting the cyclooxygenases (COX1/2) responsible for the enzymatic conversion of AA to eicosanoids, the non-steroidal anti-inflammatory drugs are effective in relieving the pain and discomfort of dysmenorrhea¹¹.

A good anti-inflammatory activity often accompanies good antioxidant activity^{14,15}. There are two basic types of antioxidants available:

synthetic and natural ones. The synthetic antioxidants typically contain phenolic groups as the main functionality. The natural antioxidants are mostly obtained from different parts of plants and their structure diversity is much larger. They can either be the nitrogen containing compounds, such as alkaloids, chlorophyll derivatives, amines and amino acids, or phenolic compounds, such as tocopherols, flavonoids and phenolic acids. Those compounds can act as oxygen scavengers, thereby terminating the harmful activity of free radicals^{16,17}. Flavonoids are considered to be the most potent antioxidants. They can delay or inhibit the oxidation of lipids or other molecules by inhibiting the propagation of oxidative chain reactions¹⁸. There has been an increased interest in natural antioxidants from plant materials in the recent years¹⁹.

Sclerochloa dura (Linnaeus) P. Beauvois, known also as common hardgrass, belongs to family Poaceae Barnhart, which involves more than 700 genera and almost 50,000 species. It is an annual plant, with flat leaves and procumbent or erect stem. The inflorescence is crowded, one-sided series of flattened spikelets²⁰. The plant is a common inhabitant of areas with heavy traffic, e.g. along dirty roads, on play yards and walking pathways. It is widely spread in the moderate climate zone on almost all the continents on North Hemisphere and introduced in Australia as well²¹.

There are only few published papers in which this plant has been mentioned. However, none of them deals with its chemical composition or bioactivity. In most of the papers the plant has been used as a specimen for determination of efficiency of various herbicides²²⁻²⁸. Two papers discuss phylogeny of certain grasses, among them *S. dura*^{29,30} and one paper deals with identification of prolamins in cereal and grass species, including *S. dura*³¹.

The plant is traditionally used in South-East Serbia for treatment of menstrual disorders, manifested as excessive bleeding and intense pain. Professor Aleksandar Igic (Medical faculty, University of Nis, Serbia) in personal correspondence reported that in this region tea or decocts of *S. dura* have been used by women having menstrual disorders. According to subjects' statements, the symptoms have been significantly alleviated shortly after intake. The remarkable story about the health improving properties of *S. dura*, supported by the lack of published data about its chemical composition and bioactivity, was the reason to start studying this plant. Therefore, we aimed to

determine the chemical composition including free radical scavenging activity, anti-oxidant activity, total phenolic and flavonoid content of *S. dura* extract, and its ability to inhibit the release of AA. In addition we wanted to compare such properties with the ones reported for other plants reported to alleviate menstrual disorders; *Wrightia tomentosa*^{32,33} and *Dendrophthoe falcata*³⁴. The novel findings here presented, forward the plant *S. dura* as a promising natural source for alleviating inflammatory disorders, including menstrual discomfort.

Experimental

Plant material

Sclerochloa dura (whole plant) was collected in June-July 2009 from the city of Nis, along the river bank near Gabrovacka reka creek in Serbia. The plant was identified by Bojan Zlatkovic from the Department of Biology and Ecology, University of Nis, Serbia. A specimen of the identified plant was deposited in the Herbarium of Faculty of Science and Mathematics (HMN) University of Nis, Serbia (voucher number 6922). Total collected weight of the plant was 250g. The plant material was dried for 10 days in a dark place, with proper ventilation and at room temperature. The dried plant was kept in a closed plastic bag, at dark place and at room temperature until extraction.

Reagents and chemicals

Water used for extraction was obtained from Millipore Elix 5 water purification system, *n*-hexane was from VWR (USA) and methanol was from Fisher Scientific (UK). Recombinant human IL-1 β was from Roche (UK). Phosphate-buffered saline solution (PBS) was from Oxoid (UK). Labelled (5,6,8,9,11,12,14,15-³H)-arachidonic acid (specific activity 180-240 Ci/mmol) and liquid scintillation cocktail Ultima Gold were from NEN Perkin Elmer (USA). Dulbecco's Modified Eagle Medium (DMEM), foetal bovine serum (FBS), fatty acid-free bovine serum albumin (fBSA), gentamicin and L-glutamine were from Sigma-Aldrich (USA). Potassium acetate, sodium carbonate, 1,1-diphenyl-2-picryl-hydrazil, sodium phosphate, α -tocopherol, quercetin, ammonium molybdate, Folin-Ciocalteu reagent, pyrocatechol and aluminium nitrate were from Sigma-Aldrich (USA). Sulphuric acid and ascorbic acid were from Merck (Germany).

Extraction

Aerial parts were crushed into small pieces and extracted by refluxing with water for 20 minutes. To enhance extraction, the water extract was sonicated for 15 minutes before and after the refluxing (VWR ultrasound cleaner). After 12 h, the extract was filtered (Blue ribbon filter paper from Schleicher and Schuell) and the volume reduced on rotavapor (BÜCHI rotavapor R-200). Dry plant sample was

obtained by freeze drying (LABCONCO freeze drier model FreeZone 2.5) at -70°C for 60 h. The crude extract was successively extracted, as shown on *Scheme 1*.

The crude extracts and subsequent fractions (C fraction – water soluble, insoluble in methanol, D fraction – methanol extract of crude; water soluble as well) were prepared from *S. dura*. The crude extract was tested for anti-inflammatory and antioxidant activities while the subsequent fractions were tested for anti-inflammatory activity only. The *S. dura* crude extract and related fractions were aliquoted in sterile glass vials and stored protected from light at 4°C prior to use. The *n*-hexane fraction (H) was not tested for anti-inflammatory activity due to the harmful effect of *n*-hexane to cells.

Culture and treatment of SW982 cells

The human fibroblastlike synoviocyte cell line SW982 was purchased from ATCC (UK) sub-cultured bi-weekly by routine trypsin detachment and kept in a sub-confluent state. The cells were maintained in DMEM supplemented with 10% FBS, 0.1 mg/mL gentamicin and 0.3 mg/mL L-glutamine in a humidified 10% CO₂ atmosphere at 37°C. For AA release, 5*10⁵ cells were seeded per well in a 48-well per plate format. Cells were cultivated until 2 days post-confluency, serum starved and labelled with ³H-AA in serum-free DMEM overnight and processed at day 3 post-confluence to ensure differentiation and synchronization of the cells. The experiments were performed in serum-free DMEM in triplicates of wells and repeated three times. In all experiments, untreated cells without inducing agents or plant extract were included for unstimulated control; distilled water was included for vehicle control. Following treatments, cells were routinely observed by microscopy to monitor possible effects on cell morphology, integrity and viability.

Arachidonic acid release assay

The AA release assay determines the amount of AA released from SW982 cells stimulated with IL-1 β . AA release corresponds to the activation of PLA₂-

Research Projects

enzymes that cleave off AA in the *sn*-2 position of the phospholipid. In the presence of inhibiting compound(s), the AA release is reduced, which is taken as evidence that the compound(s) target some level in the arachidonyl cascade, such as PLA₂ enzymes⁷⁻⁹.

At 2 days post-confluency, SW982 cells were serum-starved and labelled overnight with ³H-AA (0.4 µCi/mL) in serum free DMEM. Prior to the addition of *S. dura* extract and related fractions, the cells were washed with PBS containing fBSA (2.0 mg/mL) in order to remove unincorporated radioactivity. Cells were pre-treated with various dilutions of the crude extract and subsequent fractions (0-20% extract in serum free DMEM, 1 h preincubation) followed by addition of IL-1β (10 ng/mL) to mimic an inflammatory situation. Following 4 h and 24 h of IL-1β stimulation, the supernatants were cleared of detached cells by centrifugation (13000 rpm, 10 min). The cellular release of ³H-AA was determined by liquid scintillation counting in LS 6500 Multi-Purpose Scintillation Counter, Beckman Coulter, Inc (USA). Adherent cells were dissolved in 1.0 M NaOH in order to determine incorporated ³H-AA in the cells by liquid scintillation counting. The results are given as released ³H-AA in the supernatants relative to total ³H-AA incorporated into the cells.

Total phenolic content determination

The total soluble phenolic content of the plant extract was determined with Folin-Ciocalteu reagent using pyrocatechol as a standard^{35,36}. An aliquot of 5.0 mg of the dry plant extract was dissolved in 20.0 mL of distilled water in an erlenmeyer flask. The solution was diluted to 46.0 mL by adding distilled water. One mL of Folin-Ciocalteu reagent was added to the solution and mixture was shaken vigorously. After 3 minutes 3.0 mL of 2 % sodium carbonate solution was added. The flask was covered with aluminium foil to protect the complex from possible effect of light. Flask was shaken occasionally for 2 h at room temperature. The absorbance was measured at 760 nm^{37,38} by using UV mini-1240 – Shimadzu (Tokyo, Japan) spectrophotometer. A standard curve was plotted by using pyrocatechol as a standard and the total soluble phenolic content in the extract was expressed as µg pyrocatechol equivalent according to the following equation (1):

$$Y=0.0533X+0.0994 \quad (1)$$

(Y= Absorbance and X= Concentration)

Total flavonoid content determination

The total weight of 20.0 mg dry extract was dissolved in 1.0 mL of 80% ethanol. An aliquot of 0.1 mL was taken out of it and diluted to 1.0 mL, making concentration of 2.0 mg/mL. An aliquot of 0.5 mL (1.0 mg) was taken and added to a test tube containing 4.3 mL of 80% ethanol, 0.1 mL of 1 M potassium acetate and 0.1 mL of 10% aluminium nitrate. Incubation of mixture was done at room temperature for 40 minutes. The absorbance was measured at 415 nm by using UV mini-1240 –

Shimadzu (Tokyo, Japan) spectrophotometer. The total flavonoid content in the plant extract was expressed as µg quercetin equivalents³⁹⁻⁴¹ by using the standard quercetin graph and according to the following equation (2).

$$Y=0.0494X-0.0026 \quad (2)$$

(Y= Absorbance and X= Concentration)

Anti-oxidant activity determination

The antioxidant activity of the extract was determined with phosphomolybdenum method by using α-tocopherol as a standard^{42,43}. One mg of the extract was combined with 2.0 mL of the reagent (0.6 M sulphuric acid, 28.0 mM sodium phosphate and 4.0 mM ammonium molybdate). The blank solution was prepared by mixing 2.0 mL of the reagent solution with the appropriate volume of the same solvent used to dissolve the sample. The tubes were capped and incubated in water bath at 95°C for 90 minutes. The sample and blank were left for half an hour to cool down to room temperature. The absorbance of the sample was measured against blank solution at 695 nm by using UV mini-1240 – Shimadzu (Tokyo, Japan) spectrophotometer. A tocopherol graph was plotted by using α-tocopherol as a standard and the total antioxidant activity of the plant extract was expressed as µg α-tocopherol equivalents according to the following equation (3).

$$Y=7.7686X+1.678 \quad (3)$$

(Y= Absorbance and X= Concentration)

Free radical scavenging activity

The ability of the extract to quench 1,1-diphenyl-2-picryl-hydrazil determines the free radical scavenging activity of the plant⁴⁴⁻⁴⁶. It is usually expressed as IC₅₀ value^{37,47,48} (the extract concentration required to inhibit the activity of DPPH by 50%).

Seven different dilutions of the plant extract were made in 100% ethanol: 3200 µg/mL, 1600 µg/mL, 800 µg/mL, 400 µg/mL, 200 µg/mL, 100 µg/mL and 50 µg/mL. A volume of 1.0 mL of 0.3 mM solution of DPPH was mixed with 2.5 mL of each dilution. All the solutions were left at room temperature for 30 minutes and the absorption was measured at 518 nm by using UV mini-1240 – Shimadzu (Tokyo, Japan) spectrophotometer. Negative control was prepared by mixing 2.5 mL of ethanol with 1.0 mL of DPPH. Percentage of inhibition for all dilutions was determined by the following equation (4).

$$\% \text{ inhibition} = 100 - [(Abs_{\text{sample}} - Abs_{\text{blank}}) \times 100] / Abs_{\text{control}} \quad (4)$$

(Abs_{sample} is absorbance of each dilution; Abs_{blank} is absorbance of dilutions without adding DPPH; Abs_{control} is absorbance of the solution of DPPH in ethanol.)

The graph between probit of inhibition (a unit of measurement of statistical probability base on deviations from the mean of a normal distribution) vs. log of concentration was plotted and the IC₅₀ value of the plant extract was calculated from the graph.

Results and discussion

Physical properties of the crude extract and subsequent fractions

As the traditional use of *S. dura* is reported to be drinking it as a tea, the dried plant was crushed into small pieces and extracted by refluxing with water. From 40.0 g of the dry aerial plant parts, a yield of 4.36 g (10.9%) of dark brown colored crude extract was obtained, whereas we obtained 0.48 g (10.9% relative to dry crude) of yellow colored water soluble fraction (C); 2.79 g (64.0% relative to dry crude) of dark brown colored fraction (D) soluble in both water and methanol and 0.10 g (2.3% relative to crude) of transparent hexane soluble fraction (H). In summary, about 80% of the dried plant extract was extractable by water, methanol and hexane, whereas 20% of the fraction appeared as a black, insoluble residue. The physical properties of the crude extract and the fractions obtained from it are given in the *Table 1*.

The crude extract of *S.dura* inhibits release of arachidonic acid

The *S. dura* extract is traditionally used to alleviate menstrual cramping, excessive bleeding and pain, processes known to involve eicosanoids such as PGE₂¹³, also recognized as a pro-inflammatory mediator¹. By use of AA-release assay and the SW982 cell model system, we investigated if the extract would affect availability of AA, the rate-limiting precursor for PGE₂ synthesis. As shown in *Figure 1*, crude extract of *S. dura* inhibits IL-1 β induced AA release in a dose-dependent manner, with an observed ~50% inhibition at 1.5 mg/mL at both 4 h and 24 h of stimulation. Hence, the *S. dura* extract may contain anti-convulsive and/or anti-inflammatory compounds that interfere with the arachidonic acid cascade.

The methanolic extract of *S.dura* crude extract efficiently inhibits AA-release

Having shown that the crude *S. dura* extract inhibited AA-release, we further fractionated the crude extract into water soluble fraction (C), hexane soluble fraction (H) and methanol soluble fraction (D) (Scheme 1) in an attempt to identify the active *S. dura* compound(s). Both (C) and (D) fractions were tested for bioactivity in the AA-release assay and they inhibited IL-1 α induced AA-release in a dose-dependent manner, but with different efficacy. The inhibition observed for fraction (D), where the treatments with 0.22 mg/mL, 0.11 mg/mL and 0.06 mg/mL resulted in a 97%, 91%, and 63% inhibition of AA-release, respectively, was much higher than the one observed for fraction (C) (*Figure 2A and*

Statistical analysis

All values are expressed as mean \pm SD. Cellular bioactivity data were analysed by Student's *t*-test and results were considered significant at $p < 0.05$.

Figure 2B). Also, compared to the inhibition obtained with the crude extract, the fraction (D) was far more efficient as the IC₅₀ for fraction (D) was in the range of ng/mL, not mg/mL as observed for the crude extract. The fraction (H) was not tested due to the harmful effect of *n*-hexane to cells. This indicated that most of the bioactive compound(s) responsible for the inhibition of AA-release were located in methanol soluble fraction of the crude extract.

Antioxidant activity, phenolic content, flavonoid content and free radical scavenging activity of *S.dura* crude extract

After demonstrating that the crude extract of *S. dura* is effective in inhibiting the AA-release, our next focus was the determination of antioxidant capacity of the crude extract because a good anti-inflammatory activity often accompanies good antioxidant activity^{14,15}. The antioxidant capacity determination includes the quantification of antioxidant activity, total phenolic content and total flavonoid content by linear regression method and estimation of free radical scavenging ability by DPPH method. The antioxidant activity of the crude extract of *S. dura* was 70.11 μ g equivalents of α -tocopherol, total soluble phenolic content was 34.78 μ g pyrocatechol equivalents and total soluble flavonoid content was 22.80 μ g quercetin equivalents per milligram of the plant extract (*Table 2*). The free radical scavenging activity of several concentrations of *S. dura* extract was determined. The experiment was repeated under same conditions to determine the free radical scavenging activity of ascorbic acid which was used as a standard. The IC₅₀ value for the plant extract and ascorbic acid was determined by calculating inhibition values for all used concentrations, taking probit of all inhibition values and plotting them against log of respective concentrations. The IC₅₀ value of plant extract was 846.64 μ g/mL vs 11.77 μ g/mL of ascorbic acid. The results showed that radical scavenging activity of both ascorbic acid and the plant extract was concentration dependent. In a quest to find out the antioxidant potency of *S. dura*, the obtained results were compared with the results reported in literature for aerial parts of *Dendrophthoe falcata* (Loranthaceae) and the leaf extract of *Wrightia tomentosa* (Apocynaceae) (*Table 2*). Both of these plants chosen for comparison have a traditional use for the treatment of menstrual disorders³²⁻³⁴, a similar ethnopharmacology to *S. dura*.

Research Projects

The comparison showed that *S. dura* had 4.8 times higher total soluble phenolic content, 1.3 times higher quercetin equivalent flavonoid content and 17 times higher total antioxidant activity than *W. tomentosa*⁴². The comparison of crude extracts of both plants relative to the DPPH scavenging ability of ascorbic acid showed that the extract of *W. tomentosa* was 1.6 times more potent than the extract of *S. dura*⁴². On the other hand, there is not much difference in the total soluble phenolic and flavonoid content of *S. dura* and *D. falcata*³⁴. The

limitation in comparing the antioxidant activity and free radical scavenging activity of *S. dura* and *D. falcata* was the unavailability of published results of α -tocopherol equivalent antioxidant activity and DPPH scavenging ability compared to ascorbic acid of *D. falcata*. In summary, the antioxidant capacity of *S. dura* is similar to *D. falcata* and far better than *W. tomentosa* except for free radical scavenging ability.

Conclusion

The results from the cellular testing of *S. dura* (crude extract and sub-fractions) in AA-release assay suggest that the reported pain- and discomfort relieving effects of the plant may be explained by strong inhibitory effects on the arachidonic acid cascade. By reducing the availability of AA, the synthesis of eicosanoids may be reduced accordingly. Also, the total soluble phenolic and flavonoid contents of *S. dura* are similar to *D. falcata* but higher than *W. tomentosa*. Although *S. dura* is less effective for DPPH assay, it has higher antioxidant properties compared to *W. tomentosa*.

The presence of flavonoid compounds, known by their various pharmacological activities, a considerably high antioxidant property and the fact that *S. dura* may exert anti-convulsive, anti-inflammatory and pain-relieving properties, gives reasons to believe that the plant's use in traditional medicine has a solid chemical background. Identification of active compound(s) is the next step in the study of *S. dura*, which can potentially reveal new drug candidates for various indications.

Acknowledgements

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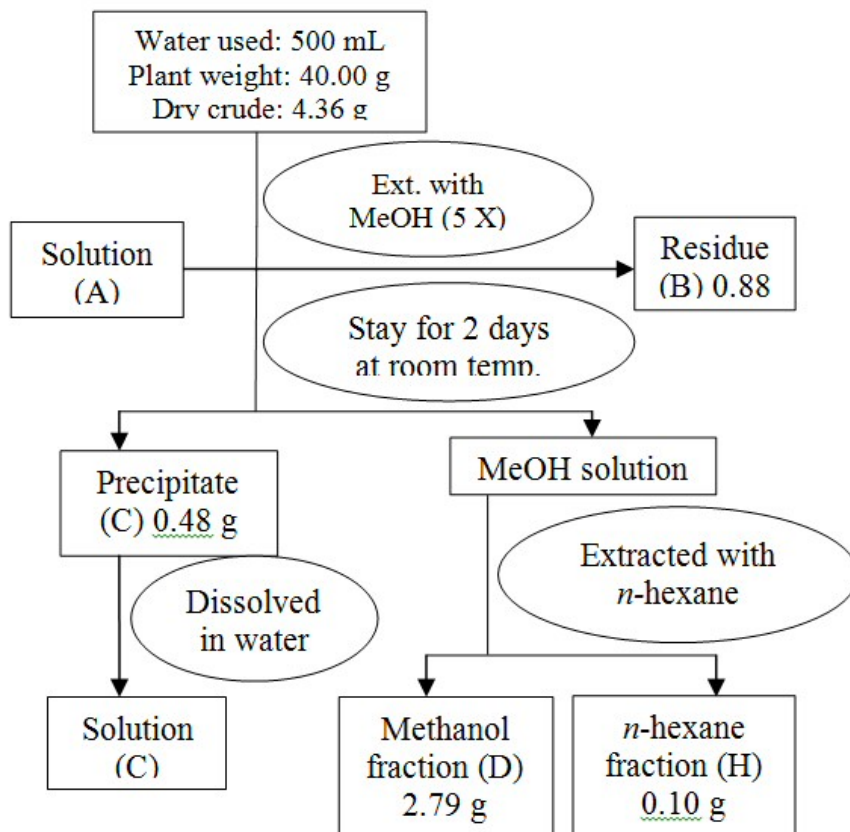
Fraction	Colour	Yield	Soluble in
Crude	Brown	10.9%	Water
C-Fraction	Yellow	11.0%*	Water
D-Fraction	Brown	64.0%*	Water and methanol
H- Fraction	Transparent	2.3%*	Hexane
(Residue)	Black	20.2%*	Insoluble

*Relative to dry crude

Table 1. Color, yield and solubility of crude extract and subsequent fractions

Plants under comparison	Total soluble phenolic content (μg pyrocatechol equivalent/mg)	Total soluble flavonoid content (μg quercetin equivalent/mg)	Total antioxidant activity (μg α -tocopherol equivalent/mg)
<i>Sclerochloa dura</i>	34.78 ± 0.375	22.80 ± 0.158	70.11 ± 0.662
<i>Wrightia tomentosa</i>	7.20 ± 0.880	16.90 ± 1.00	4.20 ± 0.03
<i>Dendrophthoe falcata</i>	38.66 ± 1.862	21.59 ± 1.09	--

Table 2. Total antioxidant activity, total soluble phenolic content and total soluble flavonoid content in the extract of *Sclerochloa dura* compared to *Dendrophthoe falcata* and *Wrightia tomentosa*



Scheme 1. Separation of crude extract of *S. dura*

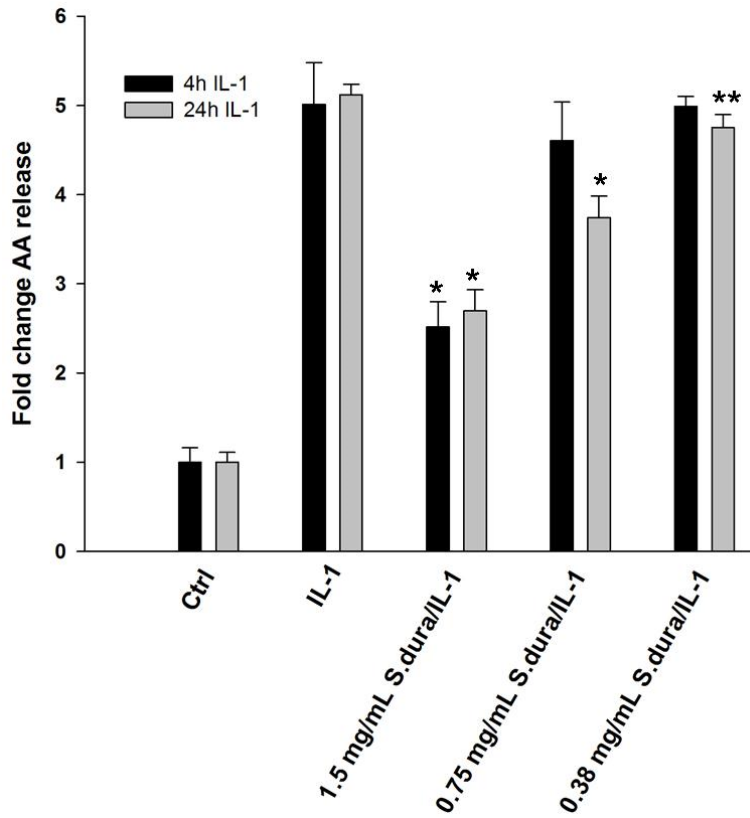


Figure 1. Crude extract of *S. dura* inhibits IL-1 (10 ng/mL) induced release of arachidonic acid in a time- and dose-dependent manner in SW982 cells. * $p < 0.001$, ** $p < 0.02$ by Students *t*-test (means \pm SD of three experiments performed in triplicates).

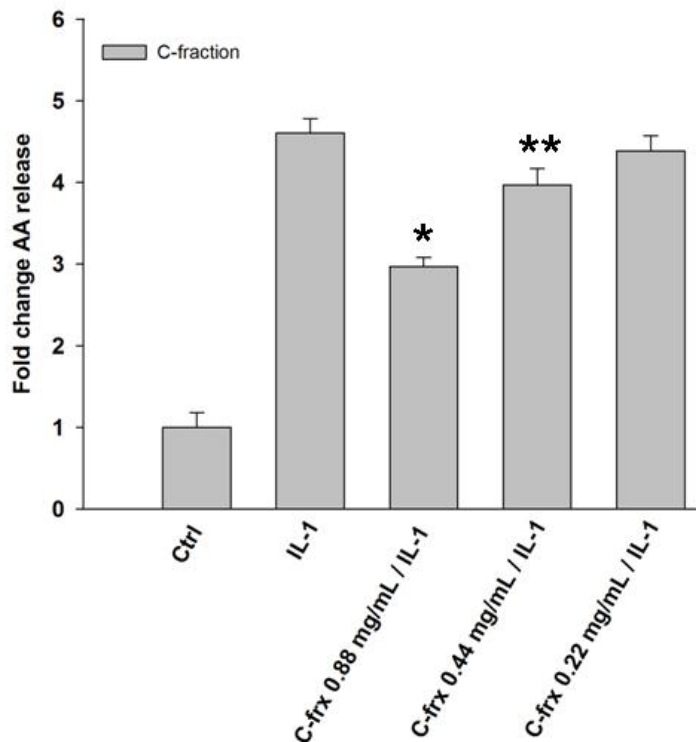


Figure 2A. Different fractions of the *S. dura* crude extract inhibit IL-1 (10 ng/mL, 24 h) induced AA-release in a dose-dependent manner, but with varying efficacy. Water soluble fraction (C) inhibits AA-release at high concentrations. * $p < 0.001$, ** $p < 0.02$ by Students *t*-test (means \pm SD of three experiments performed in triplicates).

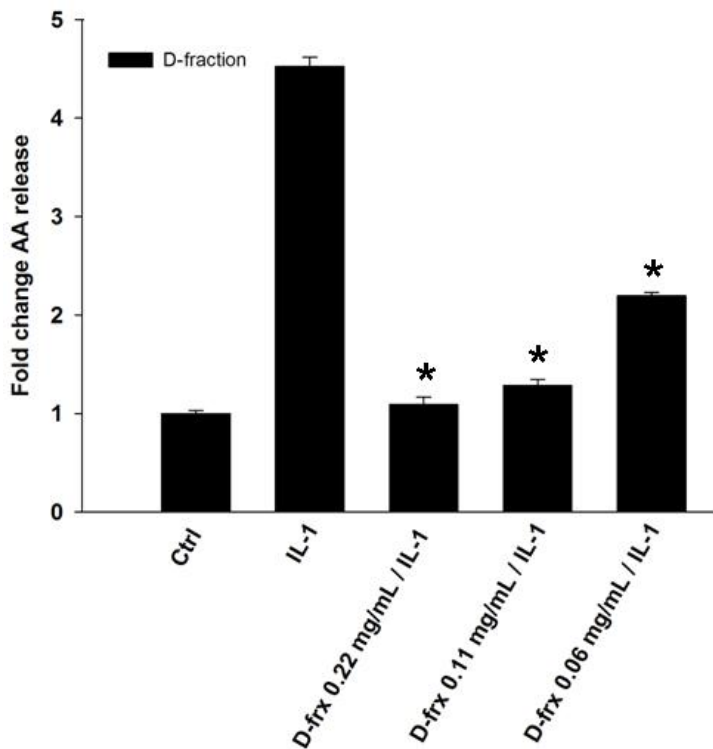


Figure 2B. Different fractions of the *S. dura* crude extract inhibit IL-1 (10 ng/mL, 24 h) induced AA-release in a dose-dependent manner, but with varying efficacy. The methanol soluble fraction (D) inhibits AA release more efficiently at lower concentrations. * $p < 0.001$ by Student's *t*-test (means \pm SD of three experiments performed in triplicates).

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Arsenic Contamination of Drinking Water in Lahore, Pakistan

It is recognised that access to clean drinking water significantly reduces incidents of water-borne diseases and that this is a basic requirement that is a necessary prerequisite to the economic and social development of developing countries. For this reason considerable effort has been expended by both governmental departments and nongovernmental agencies in providing drinking water to rural populations in many countries. However, in recent years tragic incidents in some areas, for example extensive arsenic poisoning in Bangladesh, have led to the realisation that, although tube wells are successful in providing water free of pathogens, the water supply actually contains a number of elements in concentrations that are biologically accessible and hence hazardous to human health.

One such element in particular stands out, namely arsenic because the element is ubiquitous, pernicious and very much insidious. Although

anthropological sources such as fertilisers can be important, geological sources are major contributors of contaminants. Large numbers of people have been exposed to serious arsenic poisoning from what was assumed to be clean water supplied from tube wells. The threat from arsenic applies especially to an enormous area that stretches from Bangladesh, Northern India and Pakistan and all the way down to Vietnam in South East Asia (Figure).

The source of this contamination lies in arsenic-containing minerals that are part of the Himalayas. These minerals are swept down by streams and rivers and progressively worn and broken up into particulate matter or sediment. Further breakdown eventually yields arsenic in the form of arsenic (III) and arsenic (V) oxides. These percolate down through the soil eventually reaching the aquifers that underlie this vast region.



The map shows part of the Himalayas and the area fed by its rivers, streams and aquifers. These spread arsenic-containing minerals to the full extent shown by the map

The study carried out at this department is part of an analytical and environmental project that involves collecting and analysing water samples taken from five wells located within the Municipality of Lahore, Pakistan. The samples were analysed using the facilities of the department.

The project aims to establish the levels of arsenic contamination together with some selected trace metals. Arsenic levels were found to be significantly higher than the maximum recommended by the World Health Organisation. The main source is geological.

Having found the extent of arsenic contamination, the next step is to understand the geochemistry that leads to arsenic being unlocked from the original minerals.

Our attention is directed to rationalising the role played by natural organic materials. These contain humic and fulvic acids which complex metals via their carboxyl and phenolic groups thereby breaking down minerals and hence releasing to water arsenic compounds that are now biologically available. These organic acids play an important role and it is particularly significant for the stabilities of the complexes that the oxygen-donating atoms on some of these acids are in chelating positions.

The full results and conclusions of this study will be presented in a paper which will be submitted early in 2014 and in a PhD thesis published in 2014.

Shafia Iftekhar and David G. Nicholson

Cyclotrimerization of alkynes to highly substituted benzene derivatives: Towards the synthesis of potential selective inhibitors of tyrosine kinase 2

Introduction

Multiple myeloma (MM) is the second most common hematologic cancer, accounting for about 1% of all cancer deaths worldwide.¹ The median survival time after diagnosis is 3-4 years, and there are yet no cures. Tyrosine kinase 2 (Tyk2) has been identified as a potential target for MM cancer therapy.²

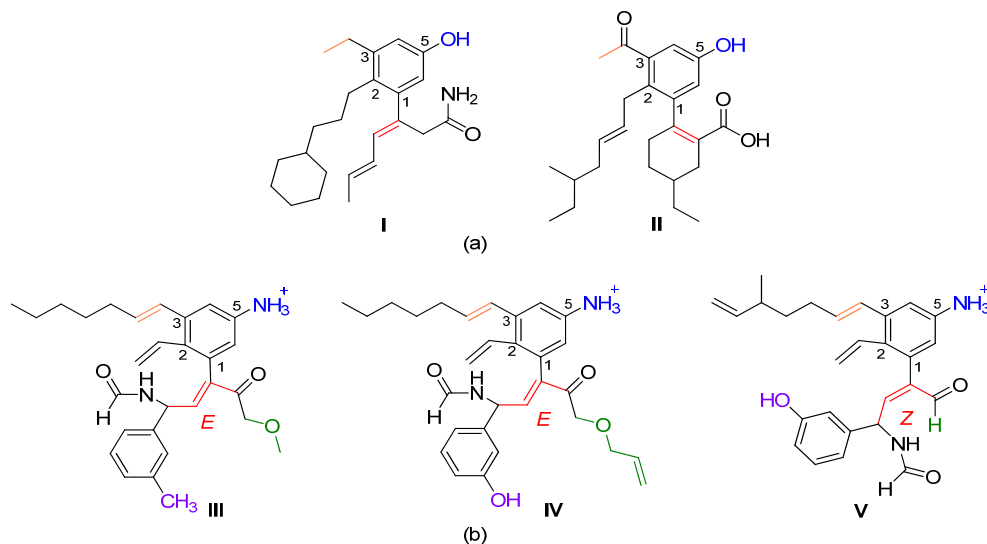
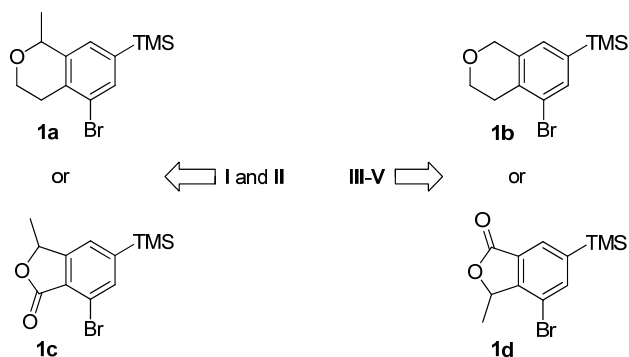


Fig. 1. Potential selective inhibitors of Tyrosine Kinase 2: I-V. (a) Structural similarities of I and II. (b) Structural similarities of III-V.

Based on computational work, Tøndel and coworkers suggested the 1,2,3,5-substituted benzene derivatives I-V as potential selective Tyk2-inhibitors (Fig. 1).^{3,4} However, I-V are not readily available and must be synthesized before their biological activity can be evaluated. Although I-V are complex molecules, structural similarities allow for common synthetic strategies. Retrosynthetic analysis pointed at compounds 1a-1d as key intermediates in the synthesis of I-V (Scheme 1).^{5,6}

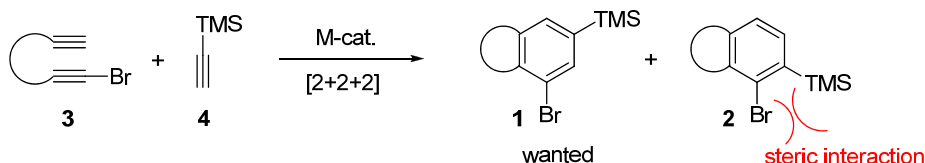


Scheme 1. Possible precursors to I-V.

The TMS (trimethylsilyl) substituent of **1** can be converted to both OH- and NH₂-groups, making **1** masked phenol- and/or aniline compounds. Several methods for such transformations exist, typically utilizing electrophilic ipso-desilylation processes.^{7,8} The bromo-substituent of **1** is a potential site for oxidative addition to palladium, and linkage of the vinylic side chains of **I-V**.

The methoxy-substituted variant of **1a** (**1a-OMe**, TMS-group replaced with an OMe-group) was prepared by eight steps from *p*-anisaldehyde in 22% total yield.⁵ Despite several high yielding steps in the synthesis of **1a-OMe**, a more direct and less time consuming route to **1** was desirable.

Transition metal catalyzed alkyne cyclotrimerization is a more straightforward strategy to highly substituted aromatic compounds from rather simple alkyne precursors.⁹⁻¹⁴ The substitution pattern in the resulting benzene product is determined by the substituents of the parent alkynes, but regioselectivity has to be controlled. Both steric- and electronic properties of catalyst and substrates might influence the selectivity.^{10,15} Today, several catalysts and good methods exist for high yielding selective alkyne cyclotrimerization reactions.⁹⁻¹⁴ Therefore, **1** might be available from the unsymmetrically bromo-substituted diynes **3** and ethynyltrimethylsilane (**4**) (Scheme 2) if the formation of regioisomer **2** can be suppressed. Alkyne-silane **4** has been used extensively by Vollhardt and coworkers in Co-mediated [2+2+2] cycloadditions.¹⁶ Both the sterically demanding TMS substituent and the polarization of the C-Si bond⁸ might influence regioselectivity in the formation of cycloaddition products.



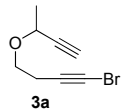
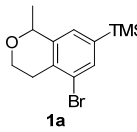
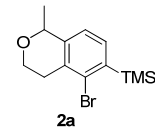
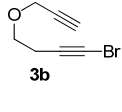
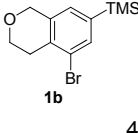
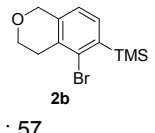
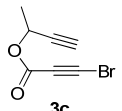
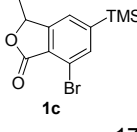
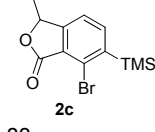
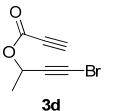
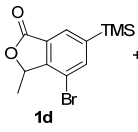
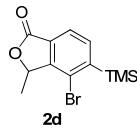
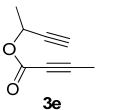
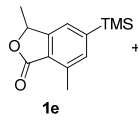
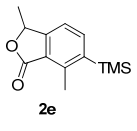
Scheme 2. The [2+2+2]-cyclotrimerization strategy for the preparation of **1**. "M": Transition metal catalyst.

Results and discussion

The diynes **3a-3e** (see Table 1) were prepared in two to three steps from commercially available starting materials.⁵ Cyclotrimerization of **3** with **4** was carried out using two different methods (A and B, Table 1).⁵ Method A refers to the cationic Rh(I)/BINAP-complex catalyzed alkyne cyclotrimerization procedure discovered by Tanaka and coworkers in 2003.^{17,18} Under mild conditions, moderate to high yields of bicyclic products from cycloadditions of 1,6-diyne and, in general less reactive 1,7-diyne, have been obtained with both electron deficient and electron rich monoalkynes.¹⁸ Cationic Rh(I)/BINAP catalyzed cycloadditions of **4** with diethyl acetylenedicarboxylate has given only moderate yields, but excellent stereoselectivity.^{17,19} In general, regioselectivity is under electronic control and depends on formation of the electronically favored rhodium metallacycle intermediate.¹⁹ Method B was developed by Yamamoto and coworkers, and employs Cp*RuCl(cod) as a pre-catalyst.^{20,21} Cycloadditions of unsymmetrical 1,6-diyne with terminal mono-alkynes in the presence of Cp*RuCl(cod) has displayed excellent selectivity of the sterically favored *meta*-products. The regioselectivity has its origin in steric interactions between the bulky Cp* ligand and the terminal alkyne substituents under formation of ruthenium metallacycle intermediates.^{20,21} An opposite *ortho*-selectivity has been observed under reactions of terminal mono-alkynes with unsymmetrically substituted diynes bearing a conjugated carbonyl group in the tether.²² The inversed regioselectivity was explained by direct electronic effects from the electron-withdrawing group *para* to the electron-donating substituent on the monoalkyne. The results obtained from reactions of **3** with **4** by both methods, are given in Table 1.⁵

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Table 1. Cyclotrimerization of unsymmetrically bromo-substituted diyne **3** with alkyne-silane **4**.⁵

Entry	3	Method ^a	% conv. 3 ^b	Products (1 : 2) ^b	% Yield ^c
1		A	100	 + 	81
2		B	100	15 : 85 90 : 10	28
3		A	100	 + 	95
4		B	58	43 : 57 90 : 10	7
5		B ^d	100	90 : 10	23
6		A	100	 + 	56
7		B ^e	100	17 : 83 97 : 3	64
8		A	100	 + 	40
9		B	70	60 : 40 77 : 23	traces
10		B ^{d,f}	100	77 : 23	42
11		B	100	 + 	97

^aMethod A: 5% [Rh(cod)₂]BF₄/BINAP, 10 equiv **4** in DCE at rt.^{17,18} Method B: 5% Cp*Ru(cod)Cl, 5 equiv **4** in DCM or DCE at rt.^{20,21} ^bDetermined by ¹H NMR analysis of the crude. ^cTotal isolated yield of **1** and **2** after column chromatography. ^d10% catalyst, 10 equiv **4**. ^eReaction finished after 30 min. ^f80 °C.

Both **3a** and **3b** reacted smoothly under the Rh-catalytic conditions applied in method A (Table 1, entries 1 and 3). High total yields of cyclotrimerization products were obtained (81 and 95% respectively). In case of **3a**, the *ortho*-isomer **2a** was formed selectively over the wanted *meta*-product **1a** (*meta:ortho* 15:85, entry 1). However, almost no selectivity (43:57) was observed under the reaction of **3b**, where the *ortho*-isomer **2b** was formed in slight excess (entry 3). Ten equivalents **4** were required to promote the wanted reaction under method A. When the amount of **4** was reduced to two equivalents, only self-trimerization products of **3a** and **3b** were observed. It should also be noted that successful cyclotrimerization by method A only was achieved when dilution (c = 0.1 M) and dropwise addition of **3** were employed. If the addition went to fast, and/or the solutions were more concentrated, considerable amounts of self-trimerization products of **3** were observed. Under the Ru-catalytic conditions in method B, the selectivity changed in favor of the wanted **1a** and **1b** (Table 1, entries 2, 4 and 5). The *meta:ortho* ratio of 9:1 was obtained in reactions of both **3a** and **3b**, indicating a lesser importance of the methyl-substituent on **3a** regarding selectivity in method B compared to method A. However, higher yields were obtained of the methyl-substituted products **1a** and **2a** (28%, entry 2) compared to the unsubstituted products **1b** and **2b** (7%, entry 4), probably due to an increased Thorpe Ingold effect²³ of **3a**. The yield of **1b/2b** was improved when a higher load of Ru-catalyst (10 mol %) and **4** (10 equivalents) were applied on **3b** (23%, entry 5), but the selectivity remained 9:1.

Only moderate yields of cyclotrimerization products were obtained when applying method A on **3c** and **3d** (Table 1, entries 6 and 8), and formation of side products were observed by TLC and ^1H NMR-analyses of the crude. A 17:83 mixture of **1c** and **2c** was obtained from **3c** in 56% isolated yield (entry 6). Selectivity in slight favour of **1d** over **2d** was observed from the reaction of **3d**, where a 60:40 mixture of products were isolated in 40% yield (entry 8). More contrasting results on both reactivity and selectivity were observed for the cyclotrimerization of **3c** compared to **3d** by method B (Table 1, entries 7, 9 and 10). While **3c** reacted completely after 30 min (entry 7), **3d** needed elevated temperature (80 °C) and higher load of both Ru-catalyst (10 mol %) and **4** (10 equivalents) to react completely (compare entry 9 and 10). An excellent selectivity (97:3) from the reaction of **3c** was observed, and the wanted meta-product **1c** was isolated as a sole product in 64%. The reactions of **3d** gave a moderate selectivity in favor of **1d** over **2d** (77:23), and a total yield of 46%.

To illustrate the significance of the diyne bromo-substituent on the reaction outcome, the bromo-substituent of **3c** was replaced with a methyl group (**3e**). Cyclotrimerization of **3e** with **4** by method B gave excellent *meta*-selectivity (97:3), and the product **1e** was isolated as a sole product in 97% yield (Table 1, entry 11).

Conclusion

Cyclotrimerization of unsymmetrically bromo-substituted diynes **3a-3d** with ethynyltrimethylsilane (**4**) has been examined as a key step for the preparation of intermediates **1a-1d** in the total synthesis of **I-V** (Fig 1). The cationic Rh/BINAP catalyzed procedure developed by Tanaka (method A) gave moderate to excellent total yields of cyclotrimerization products (**1+2**), but the regioselectivity was in general favoring the *ortho*-isomers **2**. Using Yamamoto's method with Cp*RuCl(cod) as a pre-catalyst (method B), the regioselectivity shifted towards the *meta*-isomers **1**, but the isolated yields were in general lower. The best result regarding both yield and selectivity was obtained from the Ru-catalyzed cyclotrimerization of diyne **3c**, which gave **1c** as a sole product in 64% isolated yield. A Ru-catalyzed test reaction with the methyl-substituted analogue **3e** gave **1e** in 97% yield, indicating that the bromo-substituted diynes might be labile under the reaction conditions.

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Silje Melnes, Annette Bayer, Odd R. Gautun

Bioorganic chemistry group: Structure-activity study leading to identification of a highly active thienopyrimidine based EGFR inhibitor

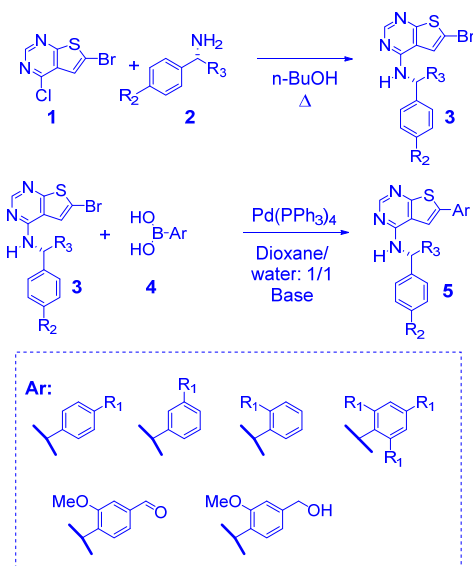
Introduction

Epidermal growth factor receptor tyrosine kinase (EGFR-TK) is one of the more important targets in small molecular cancer therapy.^{1, 2} Based on the thieno[2,3-*d*]pyrimidine scaffold, a series of new 4-amino-6-aryl thienopyrimidines have been prepared and evaluated as EGFR tyrosine kinase inhibitors.

Organic chemistry

In our previous effort for making pyrrolopyrimidine based molecules,³⁻⁵ the strategy used was not suited for efficient study of structural variations in the 6-aryl group.

Thus, a key point in the optimisation of EGFR-TK inhibitory properties has been to develop chemistry to and utilise 6-bromo-4-chloro-thieno[2,3-*d*]pyrimidine (**1**) as a late stage precursor. Compound **1** can in two or three robust transformations yield new derivatives with minimal effort. The chemistry is shown in Scheme 1.



Scheme 1. Synthesis of the thienopyrimidines.⁶

Optimisation of EGFR-TK inhibitory activity

A step-wise approach was used where substituent effects in the two sub-fragments were studied separately.

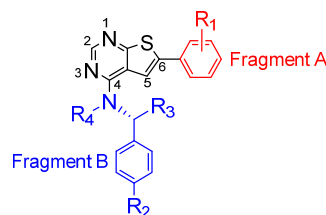


Figure 1. Optimisation plan for thienopyrimidines

Fragment A

Twenty derivatives with variations in the 6-aryl group were made and tested. The most interesting for optimisation of EGFR-TK potency are shown in Figure 2.

	CH ₂ OH	OH	OMe	Me
<i>para</i>	 7 nM (<i>R</i>)- 5e	 92 nM (<i>R</i>)- 5b	 54 nM (<i>R</i>)- 5d	 113 nM (<i>R</i>)- 5f
<i>meta</i>	 9 nM (<i>R</i>)- 5i	 46 nM (<i>R</i>)- 5j	 37 nM (<i>R</i>)- 5k	 78 nM (<i>R</i>)- 5m
<i>ortho</i>	 38 nM (<i>R</i>)- 5q	 35 nM (<i>R</i>)- 5n	 9 nM (<i>R</i>)- 5p	 153 nM (<i>R</i>)- 5r

Figure 2. IC₅₀ values (nM) of upon variation of fragment A.

Fragment B

Thirteen derivatives containing variations in fragment B were initially synthesised and tested, Figure 3. The steric bulk of the R₃ group was of minor importance for potency, while a hot spot interaction can be reached with a hydroxymethyl substituent at the stereocentre.

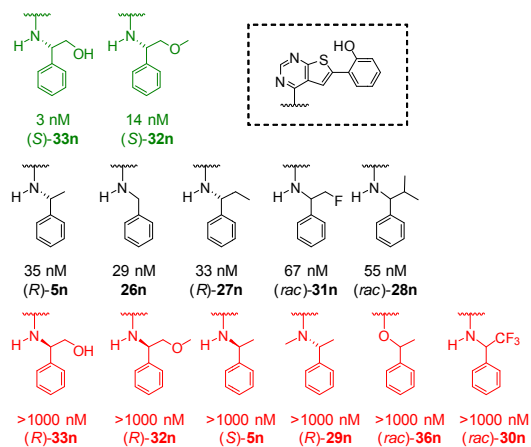


Figure 3. Investigation effect of Fragment B on EGFR-TK inhibitory properties. IC_{50} values are given in nM.

Combining active fragments

To investigate if more active compounds could be developed, the favourable substitution patterns identified were combined into new compounds, see Figure 4.

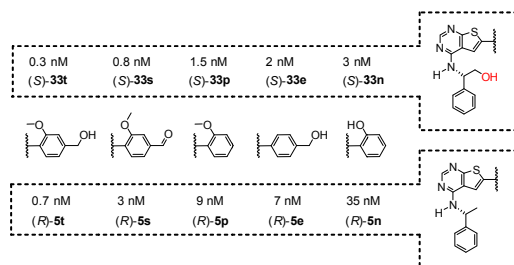


Figure 4. EGFR-TK inhibitory activity (IC_{50} nM) by combining active fragments.

Three compounds were identified as highly potent (<1 nM), of which the most active, compound (S)-33t, showed a 200 fold improvement in IC_{50} as compared to the starting point (R)-5a. Moreover, in every case the combination strategy was successful for improving the potency.

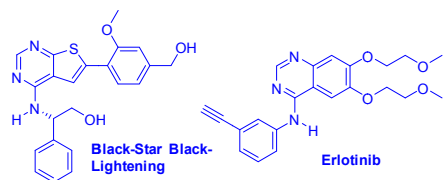


Figure 5. Structure of Erlotinib and the developed compound.

The developed compound “Black-Star Black-Lightening” was found more efficient than the commercial drug Erlotinib (Figure 5) in enzymatic assays towards the wild-type receptor and two mutants.

Molecular modelling indicates that the high EGFR-TK enzymatic inhibition potential is due to multiple directional polar interactions exerted by the additional substituents, Figure 6.

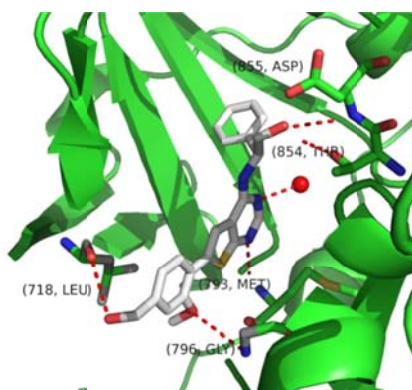


Figure 6. Docked structure of “Black-Star Black-Lightening” in EGFR. Polar interactions and hydrogen bonds towards Leu718, Met793, Thr854 and Gly796 are highlighted.

Cell assay

The best compound was first verified very active in Ba/F3 cell models, and further tested towards six other cancer cell lines: A-431 (epidermal), C-33A (cervix carcinoma), CAL-27 (tongue carcinoma), FaDu (hypopharynx carcinoma), AU-565 (breast adenocarcinoma) and NCI-H82 (a small cell lung carcinoma), see Table 1.

Table 1. Activity, IC_{50} (μ M), of “Black-Star Black-Lightening” and Erlotinib towards six cancer cell models.

Cell line	Erlotinib IC_{50} (μ M)	Black-Star B.- Lightening IC_{50} (μ M)
A-431	0.4 \pm 0.0	1.1 \pm 0.3
C-33A	0.9 \pm 0.0	1.6 \pm 0.1
CAL-27	1.3 \pm 0.6	2.8 \pm 1.4
FaDu	18 \pm 6	43 \pm 6
AU-565	3.3 \pm 0.6	6.3 \pm 0.4
NCI-H82	>20	10.9 \pm 0.2

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Black-Star Black-Lightening proved to have activity in all cell lines. However, the cellular potency of the developed EGFR-TK inhibitor was generally lower than Erlotinib. Based on the comparable EGFR enzymatic inhibitory profile, and the Ba/F3 EGFR-L858R cell model assay, this is most likely due to other cytotoxic effects caused by Erlotinib, rather than differences in drug-like properties. Anyhow, these studies identify thienopyrimidines as drug leads and reveal important structure activity relationships useful in other setting. A patent has been filed for this work. The full article is published in European Journal of Medicinal Chemistry.⁷

Acknowledgement

Professor Geir Bjørkøy (St. Olavs/HIST) and co-workers is acknowledged for taking on the cell studies. Jin Han is thanked for synthesis of an oxygenated analogue. Anders Jahres foundation is acknowledged for financial support.

Two master students have contributed to part of this work: Ellen Martine Skjønsfjell and Synne Larsen.

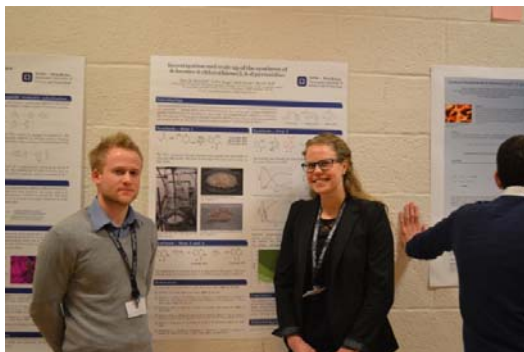


Figure 7. Steffen Bugge and Ellen Martine Skjønsfjell at OKV-2013. Ellen Martine Skjønsfjell made contribution to scale-up of the key building block 6-bromo-4-chlorothieno[2,3-d]pyrimidine (1).



Figure 8. Synne Larsen made contributions by synthesising fluoro containing thienopyrimidines.

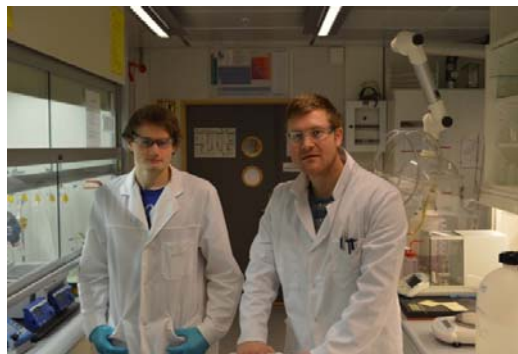


Figure 9. PhD student Svein Jacob Kaspersen (right) discussing Suzuki-coupling with Master student Kent-Ove Kragseth Sylte.

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A crowd of mallard ducks by the riverbank in february

Honours, Extracurricular activities, Participation in Courses, Conferences, Lectures, and Study Visits

B. Alsberg

Section Leader, Applied Theoretical Chemistry Group, Department of Chemistry, NTNU.

M. Ardelan

Seminar. Co-author of lecture. The Cintera Project. Havet og kystens forskningsseminar; 2013-11-13 - 2013-11-14. Trondheim, Norway.

Conference. Co-author of lecture. A comparative and holistic assessment of the effects of increased aquaculture activities in Norway and in Chile: Eutrophication and stakeholder perceptions. Aquaculture conference: To the Next 40 Years of Sustainable Global Aquaculture; 2013-11-03 - 2013-11-07. Las Palmas, Spain.

T. Bakka

Conference. Co-author of poster. Synthesis and mechanistic study of tartaric acid based surfactants. Det 28. Organisk Kjemiske Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

D. Bedeaux

Conference. Co-author of lecture. Effect of compressibility in bubble formation in a closed system. Biannual Meeting of the Royal Spanish Physical Society, Valencia, Spain; 2013-07-15 - 2013-07-19.

Workshop. Co-author of lecture. Exploring the property of local equilibrium for the Gibbs surface in two-phase multi-component mixtures. Workshop on Advances in Theory and Simulation of Non-Equilibrium Systems, Imperial College, London, UK; 2013-06-26 - 2013-06-27.



The coastal express bound for Trondheim, an early morning in October

Conference. Co-author of lecture. Curvature dependence of the heat and mass transfer resistances of the surface of nano bubbles and droplets. CECAM Workshop "Heat transfer at small scales", Zaragoza, Spain; 2013-10-14 - 2013-10-16.

Conference. Co-author of lecture. Effect of compressibility in bubble formation in a closed system. The 4th International Workshop on Nanotechnology and Application IWNA 2013, Vietnam; 2013-11-14 - 2013-11-18.

Conference. Co-author of lecture. Mesoscopic non-equilibrium thermodynamic analysis of molecular motors. 4th Nordic Workshop on Statistical Physics, Stockholm, Sweden; 2013-03-19 - 2013-03-21.

Workshop. Co-author of lecture. Bridging scales with thermodynamics: From nano to macro. 4th International Workshop on Nanotechnology and Application, Vietnam; 2013-11-14 - 2013-11-17.

Conference. Co-author of poster. Simulating CO₂ Adsorption And Diffusion On A Graphite Surface. JETC 2013 12th Joint European Thermodynamics Conference, Brescia, Italy; 2013-07-01 - 2013-07-05.

Conference. Co-author of lecture. Phase Transitions in multicomponent systems at the nano-scale: The existence of a minimal bubble size. 12th Joint European conference of Thermodynamics, Brescia, Italy; 2013-07-01 - 2013-07-05.

F. Bresme

2013 Appointed to the Scientific Committee of the Faraday discussion on Nanoparticle synthesis and assembly, to be held at Argonne National Laboratory in 2015.

REF reviewer for Edinburgh Napier university

Conference co-chair: CCP5-RSC Workshop "Advances in computer simulations of non equilibrium systems", Imperial College, June 2013

Conference co-chair: Organizer workshop "Heat transfer in small scales", CECAM, Zaragoza node, October 2013.

Conference co-author poster: "Thermal orientation in nanorod suspensions", Thermodynamics 2013, (September 2013).

Conference co-author oral contribution, "Thermodynamic efficiency of molecular machines", "Advances in computer simulations of non equilibrium systems", Imperial College, June (2013)-06-16

Activities

Conference co-author oral contribution: "Thermal polarization of water", Advances in computer simulation of non equilibrium system", Imperial College, (June, 2013).

Conference co-author oral contribution, "Thermodynamic efficiency of molecular machines", Advances in computer simulation of non equilibrium system", Imperial College, (June, 2013).

Conference, co-author poster, "Thermal orientation in nanorod suspensions", Thermodynamics 2013, (September 2013).

Conference, co-author poster, "Computer simulations of Soret coefficients in aqueous solutions", Thermodynamics 2013 (September 2013).

Conference, co-author poster, "A computational investigation of cholesterol influence on phospholipid bilayers", Thermodynamics 2013 (September 2013).

Conference, author oral presentation "Computational studies of heat transfer in water", 16th International Conference on the properties of water and steam, Greenwich (September 2013).

Conference, co-author oral/poster presentation, "Computer simulation of thermophoresis in aqueous solutions", CECAM workshop on Heat transfer at small scales, Zaragoza (October 2013).

Conference, co-author oral/poster presentation, "Thermo-orientation of model nanorods", CECAM workshop on Heat transfer at small scales, Zaragoza (October 2013).

Conference, co-author oral/poster presentation, "Thermo-orientation in polar fluids", CECAM workshop on Heat transfer at small scales, Zaragoza (October 2013).

Conference, co-author oral/poster presentation, "The Thermodynamic efficiency of a thermally driven molecular machine", CECAM workshop on Heat transfer at small scales, Zaragoza (October 2013). ORAL.

Invited seminar: "Heat transfer in nanoscale interfaces and thermo-molecular effects", Universite Libre the Bruxelles, Brussels, Belgium (January 2013).

Invited lecture: Wetting Phenomena of Soft Ultrathin Films, Wetting and Capillarity in Complex Systems, International workshop, Max Plank Institute for Complex Systems, Dresden, Germany (February 2013).

Invited lecture, Computer Simulation studies of heat conduction in water: bulk and interfaces, CECAM-ZCAM Workshop on theoretical investigation of the physicochemical behaviour of water, Zaragoza (February 2013).

Invited Seminar, Heat dissipation and thermodynamic efficiency at small scales, Department of Physics, Kings College London, UK (May 2013).

Invited lecture, Thermal gradients in biology, 12th Joint European Thermodynamics Conference, JETC 2013, Brescia, Italy (June 2013) (** Invited Panellist, top international meeting in Thermodynamics).

Invited lecture, Computer simulation studies of heat conduction in water, 7th International Discussion Meeting on Relaxations in Complex Systems, Barcelona (July 2013). (** attended by over 700 delegates, and devoted to complex systems).

Invited Seminar, "Thermal gradients at small scales: from thermal orientation to molecular pumps", Department of Chemistry, Oxford University, (November 2013).

Invited lecture, F. Bresme, Soft interfaces without thermal fluctuations", 3rd conference on Advances of Colloid materials", Granada (October 2013).

Invited Lecture "Thermal transport at the nanoscale" at the Telluride Science Research Centre, Colorado (June 2013). Could not attend due to organization of the conference: Advances in theory and simulation of non equilibrium systems, London, (June 2013).

S. Bugge

Conference. Co-author of poster. Structure-activity study of thienopyrimidines as EGFR tyrosine kinase inhibitors. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Investigation and scale up of the synthesis of 6-bromo-4-chlorothieno[2,3-d]pyrimidine. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Route selection in the synthesis of C-4 and C-6 substituted thienopyrimidines. 14th Tetrahedron Symposium; 2013-06-25 - 2013.06.28. Vienna, Austria.

Conference. Co-author of lecture. Pyrrolopyrimidines as Potential EGFR Kinase Inhibitors. The 24. International Society of Heterocyclic Chemistry Congress; 2013-09-08 - 2013-09-13. Shanghai, China.

O. Burheim

Conference. Co-author of lecture. Measured Reversible Single Electrode Heat Effects of a PEMFC. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.



The research vessel of The NTNU, Gunnerus

Conference. Co-author of lecture. Ageing, Thermal Conductivity, Water Management and PTFE Content of Porous Transport Layers for the PEMFC. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.

Conference. Co-author of lecture. Thermal Conductivity of the Micro Porous Layer (MPL) Used for the PEMFC. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.

Conference. Co-author of lecture. Reverse Electrodialysis (RED) - A Renewable Energy Source for Hydrogen Production. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.

Conference. Co-author of lecture. Thermal Conductivity of MPL and corresponding temperature profiles for the PEMFC. 3rd Zing Hydrogen & Fuel Cells Conference; 2013-07-01 - 2013-07-04.

Conference. Co-author of lecture. Thermal Conductivity, Heat Sources and Temperature Profiles of Li-ion Secondary Batteries. Electrochemical Society fall meeting; 2013-10-27 - 2013-11-01. San Francisco, USA.

Conference. Co-author of lecture. Thermoelectric cells with molten carbonate electrolytes. Molten Salt Discussion Group Christmas Meeting; 2013-12-16. Royal Chemistry, London, UK.

K.L. Bøyesen

Secretary for Trondheim branch of The Norwegian Chemical Society.

Conference. Co-author of poster. Determination of the Synergistic Effect of Copper and Vanadium Deposited on AlPO-5 for the Selective Oxidation of Propene. European Materials Research Society Spring Meeting 2013-Advances in the characterization of functional materials under relevant process conditions; 2013-05-27 - 2013-05-31. Strasbourg, France.

Conference. Co-author of lecture. Exposing the Synergistic Effect between Copper and Vanadium in AlPO-5 during Selective Oxidation of Propene.

Norwegian Catalysis Symposium 2013; 2013-12-02 - 2013-12-03. Trondheim, Norway.

Conference. Co-author of lecture. Exposing the synergistic effect between copper and vanadium in AlPO-5 during selective oxidation of propene. 3rd national meeting on inorganic and materials chemistry; 2013-10-10 - 2013-10-11. Trondheim, Norway.

Board member, BioStruct research training programme.

N. Davari

Conference. Co-author of poster. Ionization potential in high electric fields via constrained density functional theory. Very Accurate and Large Computations and Applications 2013; 2013-06-09 - 2013-06-12. Fevik, Norway.

Conference. Co-author of poster. Field-Dependent Ionization Potentials and Excitation Energies of Molecules of Relevance for Electrically Insulating Liquids. 2013 Annual Report Conference on Electrical Insulation and Dielectric Phenomena; 2013-10-20 - 2013-10-23. Shenzhen, China.

A. Fiksdahl

Conference. Co-author of poster. Gold(I) Catalyzed [5+2] Cycloaddition Reaction of Propargyl Acetal and Imines. 28. Organisk kjemisk Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of lecture. Gold(I)Catalyzed Cycloadditions of Propargyl Acetals. Organisk Kjemisk Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Member of "Det Kongelige Norske Vitenskapers Selskap" (DKNVS); (2010-).

NTNU's board member of "Anders Jahres Fond" (2010 -).

Member of expert committee, Frinatek, The Research Council of Norway.

Board member of Catalysis and organic synthetic chemistry research program, KOSK II, The Research Council of Norway.

Secretary of board, the Group of Organic Chemistry of the Norwegian Chemical Society.

Board member, "Lundgrens enkes fond", NTNU.

Member of expert committee for evaluation of applicants to post doc position at the Department of Pharmacy, University of Tromsø, Norway.

Activities

Member of assessment committee for phd candidate at the University of Oslo, Norway (supervisor: professor Mats Tilset).

Referee for miscellaneous journals.

T.P. Flaten

Conference. Co-author of poster. Do copper and iron cause demyelination?. 10th Nordic Symposium on Trace and Mineral Elements in Health and Disease; 2013-08-25 - 2013-08-29. Loen, Norway.

Conference. Co-author of lecture. Do cadmium and lead in drinking water increase the risk of hip fracture? A NOREPOS study. 10th Nordic Symposium on Trace and Mineral Elements in Health and Disease; 2013-08-25 - 2013-08-29. Loen, Norway.

Editor, Norsk Epidemiologi ((Norwegian Journal of Epidemiology).

Board member, The Committee for Geomedicine of the Norwegian Academy of Science and Letters.

Board member, Norwegian Chemical Society, Trondheim Branch.

Board member, Programme board for Environmental Exposures and Health Outcomes, The Norwegian Research Council.

Councilor, International Society for Trace Element Research in Humans (ISTERH).

S. Forselv

Conference. Co-author of poster. In-situ FTIR deactivation studies of methanol to hydrocarbons reactions over H-y, H-beta, and H-zsm-5 zeolites. 5th International Symposium Advanced Micro- and Mesoporous Materials; 2013-09-06 - 2013-09-09.

Workshop. Co-author of lecture. Infrared spectroscopic characterization of H-ITQ-7 zeolites. Workshop on Layered Materials; 2013-09-11 - 2103-09-14.

O.R. Gautun

Conference. Co-author of poster. Synthesis and mechanistic study of tartaric acid based surfactants. Det 28. Organisk Kjemiske Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Mechanistic investigation of the thermally isomerized products from monoctylammonium tartrate. Komppa Symposium - 110 Years of Natural Product Synthesis; 2013-06-24 - 2013-06-26. Espoo, Finland.

Section leader, organic chemistry group, department of chemistry, NTNU (autumn semester)

Member of NFRs committee for marine bioprospecting and organic synthesis.

K.F. Gebremariam

Conference. Lecture. Physicochemical investigation of the wall paintings of Petros Paulos Church, Ethiopia. XXXVIII Colloquium Spectroscopicum Internationale; 2013-06-17 - 2013-06-20. Tromsø, Norway.

Conference. Lecture. Technical investigation of the murals of Abuna Yemata Guh Church in Ethiopia. 17th Euroanalysis 2013, the European Conference on Analytical Chemistry; 2013-08-25 - 2013-08-29. Warsaw, Poland.

Seminar. Co-author of lecture. Church arts and AMS dating, Ethiopia. Kvikklunnsj 2013; 2013-11-29 - 2013-11-29. NTNU University Museum.

A. Gerontas

Big Science and Research Technology; an Introduction; 1st SCALES meeting, Thuir, France; 2013-03-13 – 2013-03-20.

High Performance Liquid Chromatography and Chemical Practice; the effects of automated high-speed separation in analysis. 9th International Conference in the History of Chemistry, 2013-08-21 - 2013-08-24. 9th ICHC 2013, Book of Abstracts, Uni Uppsala-Svenska Kemistsamfundet-EuCheMS.

Lecture. On the history of HPLC - bridging chemistry and biology. Lecture at the Dep. of Biotechnology, NTNU, Norway; 2013-10-09.

J. Han

Conference. Co-author of poster. Identifying mild coupling conditions for fluorinated alcohols. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.



The small craft harbour in Nidelva

E. Hjertenæs

Seminar. Co-author of lecture. Atomic simulations in DuraMat. DuraMat group meeting; 2013-09-24 - 2013-09-25. Elkem carbon, Kristiansand, Norway.

Conference. Co-author of poster. Quantum chemical investigations of sodium diffusion through graphite. Very Accurate and Large Computations and Applications; 2013-06-09 - 2013-06-12. Fevik, Norway.

Conference. Co-author of lecture. Multi-level Coupled Cluster Models. VALCA2013-Very accurate and large computations and applications 2013; 2013-06-09 - 2013-06-12. Fevik, Norway.

B.H. Hoff

Conference. Co-author of poster. Structure-activity study of thienopyrimidines as EGFR tyrosine kinase inhibitors. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Identifying mild coupling conditions for fluorinated alcohols. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Investigation of the synthesis of 6-iodo-4-chloropropolo[2,3-d]pyrimidine. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Investigation and scale up of the synthesis of 6-bromo-4-chlorothieno[2,3-d]pyrimidine. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Popular science lecture. Behandling av kreft: fra brennjern til målrettet kreftterapi. NKS møte Trondhjems avdeling; 2013-10-29 - 2013-10-29. NTNU.

Newspaper interview. Gullegg til forsker fra Nesna. Rana Blad, Mo i Rana, Norway, 2013-05-06.

Newspaper interview. Vant pris for forskning på kreft. Helgelands Blad, Sandnessjøen, Norway, 2013-05-10.



The lighthouse at Skansen

Conference. Co-author of lecture. Pyrrolopyrimidines as Potential EGFR Kinase Inhibitors. The 24. International Society of Heterocyclic Chemistry Congress; 2013-09-08 - 2013-09-13. Shanghai, China.

N. Iqbal

Conference. Co-author of poster. Gold(I) Catalyzed [5+2] Cycloaddition Reaction of Propargyl Acetal and Imines. 28. Organisk kjemisk Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of lecture. Gold(I)Catalyzed Cycloadditions of Propargyl Acetals. Organisk Kjemisk Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

E. Jacobsen

Seminar. Popular science lecture. Fra industrikjemiker til akademiker-Et arbeidsliv i labfrakk. Motivator-god kjemi; 2013-03-12 - 2013-03-12. Volvox-Alkymisten, NTNU, Norway.

Radio interview. Uillustrert vitenskap. Parabener i kosmetikk. Radio Revolt [Radio] 2013-11-14. Trondheim, Norway.

Conference. Invited lecture. Antiepileptic Drug (R)-Stiripentol by Lipase Catalysis. Drug Discovery & Therapy World Congress 2013; 2013-06-03 - 2013-06-06. Boston, USA.

Chemistry academic lay judge, Gulating lagmannsrett, Bergen, case no. 11-060302, January 7. to February 15. 2013.

Referee for one or more manuscripts in the following scientific periodicals, in 2013: Energies, Journal of Biotechnology, Journal of Molecular Catalysis B: Enzymatic, Biocatalysis and Biotransformation, Enzyme engineering, Applied Microbiology and Biotechnology.

S.J. Kaspersen

Conference. Co-author of poster. Structure-activity study of thienopyrimidines as EGFR tyrosine kinase inhibitors. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Investigation of the synthesis of 6-iodo-4-chloropropolo[2,3-d]pyrimidine. Det 28. Organisk kjemiske vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Newspaper interview. En million til mandalitt. I-a.no, Lindesnes, Norway, 2013-07-01.

Newspaper interview. La gullegget med kreftforskning. Fedrelandsvennen, Kristiansand, Norway, 2013-05-12.

Activities

Conference. Co-author of lecture. Pyrrolopyrimidines as Potential EGFR Kinase Inhibitors. The 24. International Society of Heterocyclic Chemistry Congress; 2013-09-08 - 2013-09-13. Shanghai, China.

S. Kjelstrup

Conference. Co-author of lecture. Effect of compressibility in bubble formation in a closed system. Biannual Meeting of the Royal Spanish Physical Society, Valencia, Spain; 2013-07-15 - 2013-07-19.

Workshop. Co-author of lecture. Exploring the property of local equilibrium for the Gibbs surface in two-phase multi-component mixtures. Workshop on Advances in Theory and Simulation of Non-Equilibrium Systems, Imperial College, London, UK; 2013-06-26 - 2013-06-27.

Conference. Co-author of lecture. Curvature dependence of the heat and mass transfer resistances of the surface of nano bubbles and droplets. CECAM Workshop "Heat transfer at small scales", Zaragoza, Spain; 2013-10-14 - 2013-10-16.

Conference. Co-author of lecture. Effect of compressibility in bubble formation in a closed system. The 4th International Workshop on Nanotechnology and Application IWNA 2013, Vietnam; 2013-11-14 - 2013-11-18.

Conference. Co-author of lecture. Measured Reversible Single Electrode Heat Effects of a PEMFC. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.

Conference. Co-author of lecture. Ageing, Thermal Conductivity, Water Management and PTFE Content of Porous Transport Layers for the PEMFC. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.

Conference. Co-author of lecture. Reverse Electrodialysis (RED) - A Renewable Energy Source for Hydrogen Production. Hydrogen and Fuel Cells 2013; 2013-06-16 - 2013-06-19.

Conference. Co-author of lecture. Thermoelectric cells with molten carbonate electrolytes. Molten Salt Discussion Group Christmas Meeting; 2013-12-16. Royal Chemistry, London, UK.

Invited lecture. A thermodynamic description of molecular motors. Distinguished iNano Lecture; 2013-04-11 - 2013-04-12. University of Århus, Denmark.

Radio programme. Participant. Her er verdens mest effektive varmpumpe. NRK Nord-Norge [Radio] 2013-01-29.

Newspaper paragraph. Her er verdens mest effektive varmpumpe. Aftenposten, Oslo [Avis] 2013-01-29.



The northernmost tramline in the world, an evening in December

Invited lecture. Non-equilibrium thermodynamics: A versatile theory. Lunch seminar; 2013-07-28. Technisch Nederlands Onderzoek. Delft, Netherlands.

Workshop. Lecture. Thermal osmosis and thermoelectric Potentials in polymer electrolyte fuel cell membrane materials. Heat transfer at small scales; 2013-10-14 - 2013-10-16. Zaragoza, Spain.

Workshop. Lecture. Thermal osmosis and thermoelectric potentials in polymer electrolyte fuel cell membrane materials. Water phenomena in PEM; 2013-10-03 - 2013-10-04. Department of Physics, NTNU, Trondheim, Norway.

Conference. Co-author of lecture. Mesoscopic non-equilibrium thermodynamic analysis of molecular motors. 4th Nordic Workshop on Statistical Physics, Stockholm, Sweden; 2013-03-19 - 2013-03-21.

Newspaper paragraph. Derfor er Rudolf rød på nesen. Nordlys.no, [Avis] 2013-02-11.

Workshop. Co-author of lecture. Bridging scales with thermodynamics: From nano to macro. 4th International Workshop on Nanotechnology and Application, Vietnamese National University, Vietnam; 2013-11-14 - 2013-11-17.

Conference. Co-author of poster. Simulating CO₂ Adsorption And Diffusion On A Graphite Surface. JETC 2013 12th Joint European Thermodynamics Conference, Brescia, Italy; 2013-07-01 - 2013-07-05.

Conference. Co-author of lecture. Performance indicators for evaluation of North Sea oil and gas platforms. ECOS 2013; 2013-07-16 - 2013-07-19.

Conference. Co-author of lecture. Comparative study of the sources of exergy destruction on four North Sea oil and gas platforms. ECOS 2013; 2013-07-16 - 2013-07-19.

Conference. Co-author of lecture. Phase Transitions in multicomponent systems at the nano-scale: The existence of a minimal bubble size. 12th Joint European conference of Thermodynamics, Brescia, Italy; 2013-07-01 - 2013-07-05.

Conference. Co-author of lecture. Energy efficient reactor design simplified by application of the second law of thermodynamics. 12th Joint European Thermodynamics Conference; 2013-07-01 - 2013-07-05. Brescia, Italy.

TV programme. Contributor. Innslag om MPemba-effekten og faseoverganger. Newton, NRK [TV] 2013-02-03.

H. Koch

Seminar. Co-author of lecture. Atomic simulations in DuraMat. DuraMat group meeting; 2013-09-24 - 2013-09-25. Elkem Carbon, Kristiansand, Norway.

Conference. Co-author of poster. Quantum chemical investigations of sodium diffusion through graphite. Very Accurate and Large Computations and Applications; 2013-06-09 - 2013-06-12. Fevik, Norway.

New aspects in multi-level coupled cluster theory. Invited Presentation; 2013-07-24 - 2013-07-24. ICMOL, University of Valencia.

Second quantization based methods in quantum chemistry I,II,III. Invited Presentation; 2013-01-20 - 2013-01-30. Scuola Normale Superiore, Pisa.

Conference. Co-author of lecture. Multi-level Coupled Cluster Models. VALCA2013-Very accurate and large computations and applications 2013; 2013-06-09 - 2013-06-12. Fevik, Norway.

T. Kristiansen

Conference. Co-author of lecture: Silica Aerogels; A new class of materials for catalytic purposes. 3rd national meeting on inorganic and materials chemistry; 2013-10-10 - 2013-10-11. Trondheim, Norway.

Phd defence. Silica Aerogels; A new class of materials for catalytic purposes. 2013-08-23, Trondheim, Norway.

Technical journal. Interview. Aerogel og kobber kan erstatte kostbar platina i katalysatorer. Teknisk Ukeblad, Oslo, Norway. 2013-12-03.

L. Kvittingen

Conference. Co-author of lecture. Microscale chemistry (MSC) experimentation for Ethiopian secondary schools: Development and evaluation. First African Conferences on Research in Chemistry Education; 2013-12-05 - 2013-12-07. Addis Ababa, Ethiopia.

M. Mahmoodinia

Conference. Co-author of poster. Adsorption of the platinum dimer on polyaromatic hydrocarbons by density functional theory calculations. Very Accurate and Large Computations and Applications 2013; 2013-06-09 - 2013-06-12.

A. Lykknes

Conference. Co-author of lecture. Microscale chemistry (MSC) experimentation for Ethiopian secondary schools: Development and evaluation. First African Conferences on Research in Chemistry Education; 2013-12-05 - 2013-12-07. Addis Ababa, Ethiopia.

Conference. Co-author of lecture. Ida Noddack and the fission proposal: The actor's perspective. One hundred years of the Bohr atom; 2013-06-11 - 2013-06-14. Copenhagen, Denmark.

K. Mathisen

Technical journal. Interview. Aerogel og kobber kan erstatte kostbar platina i katalysatorer. Teknisk Ukeblad, Oslo, Norway. 2013-12-03.

Workshop. Co-author of lecture. Infrared spectroscopic characterization of H-ITQ-7 zeolites. Workshop on Layered Materials; 2013-09-11 - 2013-09-14.

Conference. Co-author of poster. In-situ FTIR deactivation studies of methanol to hydrocarbons reactions over H-gamma, H-beta, and H-zsm-5 zeolites. 5th International Symposium Advanced Micro- and Mesoporous Materials; 2013-09-06 - 2013-09-09.

Ø. Mikkelsen

Conference. Popular science lecture. Foredrag om naturmiljøkjemis forskning ved IKJ/NTNU. Politikerbesøk ved NTNU; 2013-05-31.

Conference. Co-author of lecture. New knowledge and Technologies for Closed Cycle Hydroponics. GroSci 2013; 2013-06-17 - 2013-06-21. Leiden, Netherlands.

R. H. Myhre

Conference. Co-author of lecture. Multi-level Coupled Cluster Models. VALCA2013-Very accurate and large computations and applications 2013; 2013-06-09 - 2013-06-12. Fevik, Norway.

Activities

D.G. Nicholson

Conference. Co-author of poster. Correlation of molecular parameters with lipoplex structure and the transfection efficacy in pyridium-based cationic lipids. 16th Annual Meeting of the American Society for Gene & Cell Therapy; 2013-05-15 - 2013-05-18. Salt Lake City, USA.

Conference. Co-author of poster. Correlation of lipoplex morphology and transfection efficacy for pyridium-based cationic lipids by means of synchrotron radiation and X-ray diffraction. Annual reserach conference of the Qatar Science Foundation; 2013-11-24 - 2013-11-26. Doha, Qatar.

M.- L. Olivier

Head of the Department of Chemistry.

V. Partali

Conference. Co-author of poster. Polyene lipoplexes transfect retinal pigment epithelium cells. European Society of gene and Cell therapy (ESGCT); 2013-10-25 - 2013-10-28. Madrid, Spain.

Patent. Novel cationic carotenoid-based lipids for cellular nucleic acid uptake. Patentnr./Lisensnr.: US Appl. No. PCT/US13/67869 Registrert 2013-10-31.

Member of the department's approval committee for students' master degree plans.

R. Schmid

Member of the department's approval committee for students' master degree plans.

N. Simic

Patent. Co-originator. Sugar molecule. [Patent] Patentnr./Lisensnr.: UK Patent nr. GB1307331.7 Registered 2013-06-01.

E. Steinnes

Conference. Lecture. Atmospheric deposition of trace elements on the local and regional scale studied by ICP-MS analysis of moss samples. Colloquium Spectroscopicum Internationale XXXVIII; 2013-06-17 - 2013-06-20. Tromsø, Norway.

Conference. Lecture. Importance of chemical speciation in environmental studies. Applied Physico-Inorganic Chemistry; 2013-09-23 - 2013-09-26. Sevastopol, Ukraina.



This is not a medieval castle, but a hydropower plant at Leirfossen

Conference. Lecture. Metal contamination of the terrestrial environment from long-range atmospheric transport: Evidence from 35 years of research in Norway: Keynote Lecture. ECOpole 13 Conference; 2013-09-23 - 2013-09-26. Jarnoltowek, Poland.

Seminar. Lecture. Milestones in Neutron Activation analysis. XXI International Seminar on Interactions of Neutrons with Nuclei; 2013-05-20 - 2013-05-25. Alushta, Ukraina.

Conference. Lecture. Trace element exposure from atmospheric deposition. 10th Nordic Symposium on Trace and Mineral Elements in Health and Disease; 2013-08-25 - 2013-08-29. Loen, Norway.

Conference. Co-author of lecture. Is terrestrial moss a useful substrate for the assessment of atmospheric deposition of POPs? Implications from the 2010 moss survey in Norway. 26th Task Force Meeting of the ICP Vegetation; 2013-01-28 - 2013-01-31. Halmstad, Sweden.

G.M. Tesfamariam

Conference. Co-author of lecture. Microscale chemistry (MSC) experimentation for Ethiopian secondary schools: Development and evaluation. First African Conferences on Research in Chemistry Education; 2013-12-05 - 2013-12-07. Addis Ababa, Ethiopia.

T. Trinh

Conference. Co-author of lecture. Non-isothermal pyrolysis of torrefied stump – a comparative kinetics evaluation. The 5th International Conference on Applied Energy; 2013-07-01 - 2013-07-04. Pretoria, South Africa.

Guest lecture. CO₂ Capture: A Molecular Simulation Approach of Adsorption and Separation. Course Gas Cleaning and Emission Control for Stationary Combustion and Gasification; 2013-10-03.

Seminar. Lecture on Simulation labs: How to use CP2K in modelling. Simulation labs series NTNU; 2013-12-11. Trondheim, Norway.

Workshop. Lecture. Simulating mixture CO₂ / H₂ adsorption and diffusion on a graphite surface. The 4th international workshop on nanotechnology and application - IWNA 2013 14th-16th November 2013 - Vung Tau, Vietnam; 2013-11-14 - 2013-11-16.

Conference. Co-author of poster. Simulating CO₂ Adsorption And Diffusion On A Graphite Surface. JETC 2013 12th Joint European Thermodynamics Conference, Brescia, Italy; 2013-07-01 - 2013-07-05.

T. van Erp

Invited lecturer at the John van Geuns lecture series: Can we use achiral zeolites for chiral separation? Nov.14 2013, Amsterdam, the Netherlands.

Nomination for the European Science & Engineering Program (ESEP) Award which is a biannual prize granted by ExxonMobil to a young researcher (<40 y) who contributed to the field of petrochemistry; As one of the 6 laureates, invited lecturer at the ExxonMobil research day in Brussels. Nov 1 2013, Brussels, Belgium.

V. Venkatraman

Conference. Co-author of poster. Modelling Quantitative Structure Property Relationships of Organic Dyes for Photovoltaic Solar Cells. Scandinavian Symposium on Chemometrics 13 (SSC13); 2013-06-17 - 2013-06-20. Stockholm, Sweden.

Conference. Co-author of poster. QSPR-Guided de novo Design of Organic Photovoltaic Dyes. Scandinavian Symposium on Chemometrics 13 (SSC13); 2013-06-17 - 2013-06-20. Stockholm, Sweden.

S. Villa Gonzalez

Conference. Co-author of poster. Synthesis and mechanistic study of tartaric acid based surfactants. Det 28. Organisk Kjemiske Vintermøte; 2013-01-10 - 2013-01-13. Skeikampen, Norway.

Conference. Co-author of poster. Mechanistic investigation of the thermally isomerized products from monoctylammonium tartrate. Komppa Symposium - 110 Years of Natural Product Synthesis; 2013-06-24 - 2013-06-26. Espoo, Finland.

M. Voldsund

Conference. Co-author of lecture. Performance indicators for evaluation of North Sea oil and gas platforms. ECOS 2013; 2013-07-16 - 2013-07-19.

Conference. Co-author of lecture. Comparative study of the sources of exergy destruction on four North Sea oil and gas platforms. ECOS 2013; 2013-07-16 - 2013-07-19.

Ø. Wilhelmsen

Conference. Co-author of lecture. Effect of compressibility in bubble formation in a closed system. Biannual Meeting of the Royal Spanish Physical Society, Valencia, Spain; 2013-07-15 - 2013-07-19.

Conference. Co-author of lecture. Curvature dependence of the heat and mass transfer resistances of the surface of nano bubbles and droplets. CECAM Workshop "Heat transfer at small scales", Zaragoza, Spain; 2013-10-14 - 2013-10-16.

Conference. Co-author of lecture. Effect of compressibility in bubble formation in a closed system. The 4th International Workshop on Nanotechnology and Application IWNA 2013, Vietnam; 2013-11-14 - 2013-11-18.

Conference. Co-author of poster. CO₂ Dynamics - Fundamental aspects of transport and injection of CO₂ with impurities. Climit Summit; 2013-02-25 - 2013-02-26. Oslo, Norway.

Conference. Co-author of lecture. Design and Optimization of Compact Heat Exchangers in Processes used for Liquefaction of Natural Gas. International Conference on Applied Energy (ICAE 2013); 2013-07-01 - 2013-07-04. Pretoria, South Africa.

Conference. Co-author of lecture. Phase Transitions in multicomponent systems at the nano-scale: The existence of a minimal bubble size. 12th Joint European conference of Thermodynamics, Brescia, Italy; 2013-07-01 - 2013-07-05.



An angler nearby Leirfossen in Nidelva

Activities

Conference. Co-author of lecture. Energy efficient reactor design simplified by application of the second law of thermodynamics. 12th Joint European Thermodynamics Conference; 2013-07-01 - 2013-07-05. Brescia, Italy.

TV-programme. Co-contributor. Innslag om MPemba-effekten og faseoverganger. Newton, NRK, Norway. 2013-02-03.

P. – O. Åstrand

Conference. Co-author of poster. Ionization potential in high electric fields via constrained density functional theory. Very Accurate and Large Computations and Applications 2013; 2013-06-09 - 2013-06-12. Fevik, Norway.

Conference. Co-author of poster. Field-Dependent Ionization Potentials and Excitation Energies of Molecules of Relevance for Electrically Insulating Liquids. 2013 Annual Report Conference on Electrical Insulation and Dielectric Phenomena; 2013-10-20 - 2013-10-23. Shenzhen, China.

Conference. Co-author of poster. Adsorption of the platinum dimer on polyaromatic hydrocarbons by density functional theory calculations. Very Accurate and Large Computations and Applications 2013; 2013-06-09 - 2013-06-12. Fevik, Norway.

Newspaper interview. Kjemi-professor: -Glad og overrasket. Adresseavisen, Trondheim, Norway. 2013-10-10.

Meeting. Guest lecturer. The Nobel Prize in Chemistry 2013. NKS Trondheims avdelings julemøte; 2013-11-26. Trondheim, Norway.

Lecturer, Summer school on Molecular Dynamics and Chemical Kinetics, Copenhagen, August 22-28, 2013.

Leader (elected), Division of Computational Chemistry, Norwegian Chemical Society (2010-).

Panel member, Swedish Research Council (NT5 - analytical, physical and theoretical chemistry) (2013-).

Leader, NTNU Computational Science and Visualization Program (2011-2013).

Member, National Domain-specific Committee for Chemistry, NOTUR, Uninett (2013-).

Member, NTNU/SINTEF workgroup for Computational Science and Engineering (2008-2013).

Member, "Forskningsutvalget", NT faculty, NTNU (2009-2013).



A lot of masts in the inner harbour

Spring examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
KJ1020	Organic Chemistry (15)	Vassilia Partali	115/104
KJ1042	Basic Thermodynamics with Laboratory (7,5)	Signe Kjelstrup	120/100
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	Nebojsa Simic	35/30
KJ2031	Inorganic Chemistry, Advanced Course	Karina Mathisen	20/20
KJ2044	Physical Methods in Structural Chemistry (7,5)	Stian Forselv	6/6
KJ2053	Chromatography (7,5)	Rudolf Schmid	39/34
KJ2072	Environmental Chemistry (7,5)	Murat Van Ardelan	27/27
KJ2073	Analytical Environmental Chemistry (7,5)	Øyvind Mikkelsen Trond Peder Flaten	28/28
KJ2095	Experts in Teamwork - Environmental Influences on Human Health (7,5)	Trond Peder Flaten	20/20
KJ8105	Organometallic Compounds in Organic Synthesis (7,5)	Odd Reidar Gautun	1/1
KJ8205	Advanced Molecular Modelling	Per-Olof Åstrand	5/5
TKJ4130	Organic Synthesis, Laboratory (7,5)	Vassilia Partali Bård Helge Hoff	11/11
TKJ4135	Organic Synthesis, Advanced Course (7,5)	Anne Fiksdahl	16/11
TKJ4150	Organic Synthesis I (7,5)	Bård Helge Hoff Anne Fiksdahl	26/19
TKJ4170	Quantum Chemistry (7,5)	Henrik Koch	11/11
TKJ4175	Chemometrics(7,5)	Bjørn Kåre Alsberg	12/10
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	Per-Olof Åstrand	32/28
TKJ4510	Physical Chemistry, Specialization Project (15)	Bjørn Kåre Alsberg	2/2
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	1/1

Graduate Students

Autumn examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/Passed
KJ1000	General Chemistry (15)	Elisabeth Egholm Jacobsen	221/197
KJ1041	Chemical Bond, Spectroscopy and Kinetics (7,5)	Henrik Koch	90/68
KJ2050	Analytical Chemistry, Basic Course (7,5)	Øyvind Mikkelsen Florinel Gabriel Banica	57/55
KJ3022	Spectroscopic Methods in Organic Chemistry, Advanced Course (7,5)	Nebojsa Simic	22/20
KJ3050	Marine Organic Environmental Chemistry (7,5)	Øyvind Mikkelsen	11/11
KJ3053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	Bjørn Kåre Alsberg Florinel Gabriel Banica	2/2
KJ3059	Chromatography, Advanced Course	Rudolf Schmid	8/8
KJ3071	Applied Geochemistry (7,5)	Rolf Tore Ottesen	24/24
KJ3072	Advanced Aquatic Chemistry (7,5)	Trond Peder Flaten	11/11
KJ8072	Advanced Aquatic Chemistry (7,5)	Trond Peder Flaten	1/1
KJ8206	Advanced Quantum Chemical Methods (7,5)	Henrik Koch	6/6
KJ8903	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	2/2
TKJ4102	Basic Organic Chemistry	Elisabeth Egholm Jacobsen	114/100
TKJ4180	Physical Organic Chemistry (7,5)	Odd Reidar Gautun	16/12
TKJ4200	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	7/7
TKJ4205	Molecular Modelling (7,5)	Per-Olof Åstrand	20/19
TKJ4510	Physical Chemistry, Specialization Project (15)	Bjørn Kåre Alsberg	1/1
TKJ4520	Organic Chemistry, Specialization Project (15)	Odd Reidar Gautun	6/6
TKJ4525	Organic Chemistry, Specialization Course (7,5)	Anne Fiksdahl	5/5



View of Trondheim from Våttakammen

Re-sit examination

Course no.	Course title (credits)	Candidates/Passed
RFEL1001	Natural Science and World Views (7,5)	7/7
KJ1000	General Chemistry (15)	11/10
KJ1020	Organic Chemistry (15)	7/4
KJ1030	Inorganic Chemistry (15)	5/2
KJ1041	Chemical Bond Theory and Spectroscopy (7,5)	4/3
KJ1042	Basic Thermodynamics with Laboratory (7,5)	11/8
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	2/1
KJ2050	Analytical Chemistry, Basic Course (7,5)	1/0
KJ2053	Chromatography (7,5)	1/0
KJ2070	Environmental Chemistry (15)	3/2
KJ2073	Analytical Environmental Chemistry (7,5)	1/1
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	1/1
KJ3022	Spectroscopic Methods in Organic Chemistry, Advanced Course (7,5)	2/2
KJ3050	Marine Organic Environmental Chemistry (7,5)	1/1
KJ3053	Analytical Methods for Industrial- and Environmental Monitoring (7,5)	1/0
KJ8059	Chromatography, Advanced Course	1/0
KJ8100	Organic Medicinal and Pharmaceutical Chemistry (7,5)	1/1
TKJ4102	Basic Organic Chemistry(7,5)	8/5
TKJ4135	Organic Synthesis, Advanced Course (7,5)	1/1
TKJ4150	Organic Synthesis I (7,5)	1/1
TKJ4170	Quantum Chemistry (7,5)	1/1
TKJ4175	Chemometrics (7,5)	1/1
TKJ4190	Physical Chemistry, Project Work (7,5)	2/2
TKJ4215	Statistical Thermodynamics in Chemistry and Biology (7,5)	1/1

Graduate Students

Technology students

3. year (MTKJ)

Aae, Bjørn Erik Sylthe
Folkestad, Sarai Dery
Fougner, Hugo In'T Veld
Hereide, Yngve Mannsåker
Kjønstad, Eirik Fadum
Kringhaug, Henrik Holthe
Larsen, Kristin Uhlving
Lindberg, Daniel
Nguyen, Phuong Toan
Reiersølmoen, Ann Christin
Roest, Didrik Lindberg
Uggerud, Nora
Walderhaug, Martin E.

4. year (MTKJ)

Asplin, Alexander
Bekkevard, Pål Unnerud
Buene, Audun Formo
Evjen, Sigvart
Falck, Merete
Haarseth, Pia Kristine
Hansen, Ole Kudsk
Henriksen, Silje
Landsem, Elise
Ringheim, Ingvild

5. year (MTKJ)

Hauge, Hans Henrik R.
Holden, Mia Cathrine Hellandsjø
Lund, Ingvild Teigen
Moen, Ingri Ullestad
Skjelbred, Kristin Marie

Master students in progress

Chemistry (MKJ)

Aaen, Ingrid
Ali, Daniel
Benden, Tonje Fagertun
Berge, May Britt
Fauskanger, Tine Olsen
Finstad, Martin
Haugen, Ingrid Naterstad
Hirkjølen, Morten
Jakobsen, Trygve Dagsloth
Kirkemo, Fredrik Motland
Linde, Henrik
Mahmud, Zahra Galal
Nervik, Sondre
Nesbakken, Mari
Ofstad, Benedicte
Pettersen, Iselin Esp
Simensen, Jan Tore
Sjursen, Kenneth Røsvik
Slotten, Geir Andreas
Strand, Robin Viktor
Sylte, Kent-Ove Kragseth
Tveit, Erik Våland
Vestbøstad, Marie Tveit
Willumsen, Fredrik Bysting

Environmental toxicology and chemistry (MSENVITOX)

Dunnebier, Dorien Anna Engelbertha
Stankova, Radka
Vike, Kristine
Wang, Pan

Master of Science Education (MLREAL)

Baardsgaard, Margrete Marine
Børset, May
Børseth, Kristine
Ekeland, Mari Helen P.
Gjendemsjø, Eirin
Hosking, Tone
Jenssen, Ida Helena
Kirkemo, Solvor Motland
Nygard, Ingeborg
Roset, Marianne
Wallerøynet, Trude

The following Ph.d. projects are in progress

PhD-student	Working title	Supervisors
Abburu, Sailesh	Development and use of de novo design tools to find new transition metal complexes with optimal properties.	Alsberg, Bjørn K. (main superv.) Jensen, Vidar R
Badina, Aderonke	Efficient production of fuels from biomass- The use of microwave and hydrolic enzymes in processing of biomass.	Hoff, Bård Helge
Bakka, Thomas A	Synthesis of novel antibiotics inspired by marine natural products	Gautun, Odd R. (main superv.) Strøm, Morten Bøhmer Fiksdahl, Anne
Bugge, Steffen	Heteroaromatic compounds as new anticancer agents, diagnostic tools, and protozoal agents	Hoff, Bård Helge
Børset, Marit Takla	Methods to utilize waste heat in the ferro alloy industry	Kjelstrup, Signe (main superv.) Burheim, Odne Kolbeinsen, Leiv
Bøyesen, Katrine	Combined Raman, X-ray Absorption, Scattering and diffraction studies on nanoparticulate VOx species in micro and mesoporous systems for the selective oxidation of propene and propane.	Mathisen, Karina
Catelli, Emilio	Norwegian cultural heritage: A chemical perspective	Banica, Florinel (main superv.) Kvittingen, Lise
Davari, Nazanin	Molecular modeling of breakdown processes in electrically insulating liquids	Åstrand, Per-Olof (main superv.) Ingebrigtsen, Stian
Forselv, Stian	Catalytic conversion of 2nd generation biomass to liquid fuels over nanostructured hierarcial solids	Mathisen, Karina (main superv.) Svelle, Stian Bjørgen, Morten
Gebremariam, Kidane Fanta	Analytical methods for art objects investigation	Kvittingen, Lise (main superv.) Banica, Florinel
Gerontas, Apostolo	A history of the development of column chromatography: From Tswet to HPLC	Lykknes, Annette (main superv.) Hentschel, Klaus
Haghdani, Shokouh	Force field model for optical rotation in macromolecules	Åstrand, Per-Olof (main superv.) Alsberg, Bjørn K. Koch, Henrik
Han, Jin	Identification of TIE2 inhibitor for cancer treatment	Hoff, Bård H. (main superv.) Sundby, Eirik
Hjertenæs, Eirik	Quantum chemical calculations on sodium-graphite systems and development of a computational method utilizing non-orthogonal Slater Determinants	Koch, Henrik (main superv.) Andersson, Stefan

Post Graduate Students

PhD-student	Working title	Supervisors
Iftekhar, Shafia	Trace metals and natural organic matters in rivers	Berg, Torunn (main superv.) Flaten, Trond Peder Mikkelsen, Øyvind
Karlsen, Morten	Synthesis of ¹³ C-labelled standards for analysis of narcotics	Hoff, Bård Helge (main superv.) Liu, Hui-Ling
Kaspersen, Svein Jacob	New pyrrolo, thieno and furopyrimidine targeting tyrosine kinases (cancer) and protozoas synthesis and bioactivity	Hoff, Bård Helge
Løkken, Torbjørn Vegard	Analyser av vandduggpunkt og hydrokarbonduggpunkt i naturgass. (Determination of water dewpoint and hydrocarbon dewpoint in natural gas.)	Schmid, Rudolf (main superv.) Fredheim, Arne Olav
Mahmoodinia, Mehdi	Molecular modelling of the Fischer-Tropsch process	Åstrand, Per-Olof (main superv.)
Martinsen, Morten	Development of an on-line monitoring platform and procedure for rapid environmental and process monitoring of heavy oil extraction operations and industrial activity	Mikkelsen, Øyvind (main superv.) Schmid, Rudolf
Moqadam, Mahmoud	Studying silica oligomerization reactions using QuanTIS	van Erp, Titus Åstrand, Per-Olof
Myhre, Rolf Heilemann	Development and implementation of multi-level coupled cluster methods	Koch, Henrik (main superv.) Sunde, Svein
Nordløkken, Marit	Trace of elements in Norwegian deer	Berg, Torunn (main superv.) Flaten, Trond Peder Steinnes, Eiliv
Puerto, Nicolas Sanchez	Iron bioavailability to phytoplankton and its feedbacks to the biogeochemical cycling in the Mediterranean and Polar ecosystems	van Ardelan, Murat (main superv.) Olsen, Yngvar
Raju, Rajesh	Optically active amphiphiles and artificial cells	Gautun, Odd Reidar
Saepurahman	Spectroscopic studies of zeolites and zeolite facilitated oxygenate/-hydrocarbon conversion reactions	Mathisen, Karina (main superv.) Svelle, Stian
Siah, Huey-San Melanie	Gold catalysis in organic synthetic chemistry	Fiksdahl, Anne (main superv.) Gautun, Odd Reidar
Simic, Anica	Trace elements and persistent organic pollutants (POPs) in blood serum samples from the Nord-Trøndelag health study (HUNT) and the possible role of trace elements in type 2 diabetes	Flaten, Trond P. (main superv.) Midthjell, Kristian
Skorpa, Ragnhild	A thermodynamic base for reaction kinetics. Studied by non-equilibrium molecular dynamics simulations	Kjelstrup, Signe

PhD-student	Working title	Supervisors
Tesfamariam, Gebrekidan M.	Enhancing the quality and relevance of chemistry teacher training education in Ethiopia: A study of the use and impact of small-scale, low cost experiments at Mekelle University	Lykknes, Annette (main superv.) Kvittingen, Lise
Zaidi, Asma	Synthesis of highly unsaturated amino acids	Partali, Vassilia (main superv.) Sliwka, Richard
Voldsund, Mari	Entropy production in process equipment	Kjelstrup, Signe (main superv.) Ertesvåg, Ivar
Weggeberg, Hanne	Metal characterization of different size fractions of airborne particulate matter and adverse health effects in humans	Flaten, Trond P. (main superv.) Hilt, Bjørn
Wilhelmsen, Øivind	Non-equilibrium thermodynamics of phase transitions	Kjelstrup, Signe (main superv.)
Waage, Magnus	Kinetic properties of gas hydrates	Kjelstrup, Signe (main superv.) van Erp, Titus



Apple blossoms in the garden

Post Graduate Students

MSc in Chemistry

Aakre, Iselin	A Method for Rapid Localisation of Hydrocarbon Compounds on Surfaces Using Chemical Imaging and Back-Projection
Supervisor:	Professor Bjørn Kåre Alsberg
Examiners:	Dr. Ing Kay Steen Professor Øyvind Mikkelsen
Bakka, Thomas Aleksander	Synthesis and Mechanistic Studies of Optically Active Tartaric Acid Based Surfactants
Supervisors:	Associate Professor Odd Reidar Gautun Senior Engineer/Dr. Scient Susana Villa Gonzalez
Examiners:	Research Manager/Dr. Scient Huiling Liu, Chiron Professor Vassilia Partali
Blomli, Janne Yttermo	Environmental Pollutants in Electrical and Electronic Waste
Supervisors:	Professor Trond Peder Flaten Professor II/Researcher Rolf Tore Ottesen, NGU
Examiners:	Researcher Tor Erik Finne, NGU Associate Professor Rudolf Schmid
Borkowska, Zuzanna	Silicon Production Process. Energy and Exergy Analysis for Holla Silicon Plant
Supervisor:	Professor Signe Kjelstrup
Examiners:	Principal Engineer/Dr. Ing. Audun Røsjorde, Statoil Professor II Halvard Tveit, IMT
Gjesteland, Ingrid	Study of Water Quality of Recirculated Water in Aquaponic Systems. Study of speciation of selected metals and characterization of the properties of natural organic matter
Supervisors:	Professor Øyvind Mikkelsen Research Manager/Dr. Scient Åse Åtland, NIVA
Examiners:	Researcher/PhD Ole-Kristian Hess-Erga, NIVA Professor Emeritus Eiliv Steinnes Professor Øyvind Mikkelsen
Johansen, Frank Edvardsen	Stabilization of Trivalent Vanadium in Zeotypic Systems
Supervisors:	Associate Professor Karina Mathisen Senior Engineer/PhD Morten Bjørgen
Examiners:	Researcher/PhD. Camilla Nordhei, IFE Associate Professor Hilde Lea Lein
Karlsen, Silje Sæther	Impact of metals in salmon smolt. Mainly iron and copper
Supervisors:	Professor Øyvind Mikkelsen Per Brunsvik, NOFIMA
Examiners:	Professor Emeritus Knut Schrøder Associate Professor Muran van Ardelan
Kirste, Karsten Granlund	Synthesis And Characterization Of Noble Metal Nanoparticle Impregnated Metal-Organic Frameworks
Supervisors:	Associate Professor Karina Mathisen Associate Professor Odd Reidar Gautun
Examiners:	Senior Engineer/PhD Morten Bjørgen, Norsk Akkreditering Associate Professor Bård Helge Hoff

<p>Lien, Vegard Torp Supervisor: Examiners:</p>	<p>Transition metal catalyzed cyclotrimerization to new pyridine ligands for asymmetric hydrogenation Associate Professor Odd Reidar Gautun Professor Tore Lejon, UiT Associate Professor Bård Helge Hoff</p>
<p>Lindgjerdet, Per Magnus Supervisor: Examiners:</p>	<p>Organic Chemistry as a common Education Associate Professor Annette Lykknes Professor Emeritus Reidar Stølevik Professor Lise Kvittingen</p>
<p>Madland, Eva Supervisor: Examiners:</p>	<p>Extraction, Isolation and Structure Elucidation of Saponins from Herniaria incana Associate Professor Nebojsa Simic Professor Torgils Fossen, UiB Professor Vassilia Partali</p>
<p>Mikalsen, Ragni Fjellgaard Supervisors: Examiners:</p>	<p>Hydrothermal synthesis of materials for intermediate band solar cells Associate Professor Karina Mathisen Associate Professor Fride Vullum-Bruer, IMT Senior Research Scientist/PhD. Tommy Mokkelbost, SINTEF Associate Professor Turid Worren Reenaas, IFY</p>
<p>Næss, Isabel Stubberud Supervisor: Examiners:</p>	<p>The Effect of Roadwork on Stream Systems. Evaluation of Metal Levels and Speciation Studies in Areas connected to the new E6 Oslo-Trondheim Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder Professor Trond Peder Flaten</p>
<p>Ophaug, Camilla Supervisor: Examiners:</p>	<p>Speciation studies and studies of short time fluctuations for zinc and iron (and copper) in streams receiving runoffwater from pyrite mines Professor Øyvind Mikkelsen Professor Knut Schrøder Associate Professor Rudolf Schmid</p>
<p>van der Wijst, Cornelis G. Supervisors: Examiners:</p>	<p>Oxygenate conversion over protonated zeolites Associate Professor Karina Mathisen PhD-candidate Stian Forselv Senior Engineer/PhD Morten Bjørgen, Norsk Akkreditering Research Scientist/Dr. Ing.Knut Thorshaug, SINTEF Professor Magnus Rønning, IKP</p>
<p>Yttervik, Johan Hatling Supervisor: Examiners:</p>	<p>NOx Storage reduction on copper and barium containing micro- and mesoporous materials Associate Professor Karina Mathisen Associate Professor/Dr. Scient Stian Svelle, UiO Professor Magnus Rønning, IKP</p>

Post Graduate Students

MSc in Chemistry/Technology.

Dahlen, Oda Supervisor: Examiners:	The dynamics of DNA denaturation Associate Professor Titus van Erp Professor/Dr. Scient Santiago Cuesta-Lopes, University of Burgos Associate Professor Titus van Erp
Glansberg, Karin Märta Supervisors: Examiners:	Studies of the Variables Influencing the Properties of Self-polishing Antifouling Associate Professor Bård Helge Hoff Marcus Tullberg, Jotun Aslan Esmurziev, Jotun Kjartan Boman, Jotun R&D Chemist/PhD Mikael Hillgren, Jotun Associate Professor Bård Helge Hoff
Hogsnes, Morten Christian Supervisor: Examiners:	Gold(I) Catalyzed Tandem Cyclization Reactions with Propargyl Acetals Professor Anne Fiksdahl Professor Tore Lejon, UiT Professor Signe Kjelstrup
Johansen, Maren Teresa Supervisors: Examiners:	Degradation of Amines Professor Anne Fiksdahl Professor Hallvard Svendsen, IKP Associate Professor Hanna Knuutila, IKP Research Scientist/Dr. Ing. Andreas Grimstvedt, SINTEF Materials and Chemistry Professor Anne Fiksdahl
Kolstad, Aleksander Supervisor: Examiners:	Membrane processes relevant for the polymer electrolyte fuel cell Professor Signe Kjelstrup Principal Engineer/Dr. Ing Audun Røsjorde, Statoil Professor Signe Kjelstrup
Myhre, Rolf Heilemann Supervisor: Examiners:	Development and implementation of extended CC2 models Professor Henrik Koch Associate Professor/PhD Thomas Bondo Pedersen, UiO Professor Henrik Koch
Rydså, Line Supervisors: Examiners:	Scale-Up and Use of a Dihalogenated Pyrrolopyrimidine for the Preparation of New Active Tyrosine Kinase Inhibitors Associate Professor Bård Helge Hoff PhD-candidate Svein Jacob Kaspersen Researcher/PhD Tor Erik Kristensen, FFI Associate Professor Bård Helge Hoff
Skjønsvjell, Ellen Martine Supervisors: Examiners:	Synthesis of thienopyrimidines for use in cancer chemotherapy Associate Professor Bård Helge Hoff PhD-candidate Steffen Bugge Researcher/Dr. Ing. Harald Svensen, EPAX Associate Professor Bård Helge Hoff
Tveikrem, Marit Elise E. Supervisor: Examiners:	Quantum Chemical Calculations on the Physisorption of Molecular Hydrogen on N-doped Graphene Professor Henrik Koch Associate Professor/PhD Thomas Bondo Pedersen, UiO Professor Henrik Koch

MSc in Education, chemistry

<p>Grøndal, Stine Skimmeland</p> <p>Supervisor: Examiners:</p>	<p>Mapping of Metal Contamination in Sediments in Ilsvika / Fagervika. Laboratory Studies of Leaching of Metals through Capping Materials</p> <p>Professor Øyvind Mikkelsen Professor Emeritus Knut Schrøder Professor Øyvind Mikkelsen</p>
<p>Horgheim, Jorunn Bårdsnes</p> <p>Supervisor: Examiners:</p>	<p>Micronutrient Distribution in Relation to Waste Emission from Aquaculture Activities. A field study in Trondheimsfjorden</p> <p>Associate Professor Murat Van Ardelan Professor Emeritus Jon-Arne Sneli Associate Professor Murat Van Ardelan</p>
<p>Klungvik, Elina</p> <p>Supervisors: Examiners:</p>	<p>Studies and mapping of metals and natural organic matter in river Moelva, Birkenes/Lillesand and Stordalsbekken stream, Lillesand. Influence from local sources of sulphide-bearing rocks</p> <p>Professor Øyvind Mikkelsen Professor Trond Peder Flaten Professor Emeritus Knut Schrøder Professor Øyvind Mikkelsen Professor Trond Peder Flaten</p>
<p>Kronborg, Anne Ingelill E.</p> <p>Supervisors: Examiners:</p>	<p>Trace Elements in Norwegian and Polish Tea Infusions. Determined by High-Resolution Inductively Coupled Plasma Mass Spectrometry (HR ICP-MS) and Ion Selective Electrode (ISE)</p> <p>Professor Trond Peder Flaten Researcher Tomasz Ciesielski, IBI Professor Emeritus Eiliv Steinnes Professor Trond Peder Flaten Researcher Tomasz Ciesielski, IBI</p>
<p>Sandstad, Vidar</p> <p>Supervisors: Examiners:</p>	<p>Leakage of Methane and Carbon Dioxide From the Old Landfill in Steinkjer City</p> <p>Professor Trond Peder Flaten Professor II Rolf Tore Ottesen, NGU Senior Engineer Silje Salomonsen, Trondheim Kommune Professor Trond Peder Flaten Professor II Rolf Tore Ottesen, NGU</p>
<p>Skaret, Lise Bjerkestrand</p> <p>Supervisors: Examiners:</p>	<p>Potential Inhibitors of Tyrosine Kinase 2. Synthesis of Important Intermediates</p> <p>Associate Professor Odd Reidar Gautun PhD-candidate Silje Melnes Research Manager/Dr. Scient Huiling Liu, Chiron Associate Professor Odd Reidar Gautun</p>
<p>Solli, Cathrine Malvik</p> <p>Supervisor: Examiners:</p>	<p>Macronutrient Distribution in Relation to Waste Emission from Aquaculture Activities. A field study in Trondheimsfjorden</p> <p>Associate Professor Murat Van Ardelan Professor Emeritus Jon-Arne Sneli Associate Professor Murat Van Ardelan</p>

Post Graduate Students

MSc in Environmental toxicology and chemistry (MSENVITOX)

Hansen, Ailin Falkmo	Selected trace elements in undiagnosed diabetes mellitus type 2 FINDRISC\geq15 - a nested case-control study (HUNT3)
Supervisors:	Professor Trond Peder Flaten Professor Kristian Midthjell
Examiners:	Professor Emeritus Eiliv Steinnes Professor Øyvind Mikkelsen
Ramzan, Muhammad	Effect of Surface Chemistry and Physical Properties of Carbon Nanotubes on the Adsorption of Polycyclic Aromatic Hydrocarbons in Aqueous Solutions
Supervisors:	Associate Professor Rudolf Schmid Professor Øyvind Mikkelsen Research Scientist Andy Booth, SINTEF
Examiners:	Associate Professor/Dr. Scient Birte J. Sjursnes, HiØ Associate Professor Florinel G. Banica
Rusti, Elise Hermo	Urban mining. Recycling of EE-waste focusing on rare earth metals and noble metals
Supervisors:	Professor Trond Peder Flaten Professor II Rolf Tore Ottesen, NGU
Examiners:	Researcher Tor Erik Finne, NGU Associate Professor Rudolf Schmid



Hopefully, a non-toxic small stream in springtime

PhD in Chemistry, finished 2013:

<p>Bukhari, Syed Majid Trial lecture Supervisor Assessment Committee</p>	<p>Isolation and structure elucidation of anti-inflammatory compounds from <i>Sclerochloa dura</i> Drug discovery and drug development – from the discovery of a lead compound to the market Associate Professor Nebojša Simić Professor Frode Rise, Department of Chemistry, University of Oslo Professor Peter Molar, Department of Pharmacognosy, University of Pécs, Hungary Professor Vassilia Partali, Department of Chemistry, NTNU</p>
<p>Kristiansen, Tina Trial lecture Main supervisor Co-supervisor Co-supervisor Assessment Committee</p>	<p>Aerogels; a new class of materials for catalytic purposes Strategies for NOx reduction Associate Professor Karina Mathisen Professor David Nicholson, Department of Chemistry Professor Mari-Ann Einarsrud, Department of Materials Science and Engineering Professor Wendy Flavell, The University of Manchester, UK Professor Serena Margadonna, Institutt for kjemi, UiO Professor Per-Olof Åstrand, Institutt for kjemi, NTNU</p>
<p>Melnes, Silje Trial lecture: Supervisor Assessment Committee</p>	<p>Rational Drug Design. Synthetic studies toward potential selective inhibitors of tyrosine kinase 2 MIDA-Protected Boronate Esters: Properties, Synthesis and Applications in the Total Synthesis of Natural Products Associate Professor Odd Reidar Gautun Professor David Tanner, Technical University of Denmark Professor Trond Vidar Hansen, Department of Pharmaceutical Chemistry, University of Oslo Professor Anne Fiksdahl, Department of Chemistry, NTNU</p>
<p>Sandru, Eugenia-Mariana Trial lecture Main supervisor Co-supervisor Assessment Committee</p>	<p>Polyene nanoparticles Natural occurring organosulfur compounds and corresponding selenium derivatives Professor Vassilia Partali Dr. Richard Sliwka Professor Bernd Schaefer, Universität Heidelberg, Germany Professor Tibor Hianik, Comenius University in Bratislava, Slovakia Associate Professor Florinel Banica, Department of Chemistry, NTNU</p>
<p>Thvedt, Thor Håkon Krane Trial lecture Main supervisor Co-supervisor Assessment Committee</p>	<p>Synthesis of fluorinated building blocks and chiral antifungal agents Novel chemical approaches to amide formation Associate Professor Bård Helge Hoff Associate Professor Eirik Sundby Senior Lecturer Morten Grøtli, University of Gothenburg, Sweden Associate Professor Annette Bayer, University of Tromsø, Norway Associate Professor Odd Reidar Gautun, Department of Chemistry, NTNU</p>

Post Graduate Students

Student Exchange from NTNU, Department of Chemistry

Name	Specialization	Level	Institution
Hauge, Hans Henrik	MTKJ-Phys.chem	MSc, 4th yr	TUM, Germany
Leraand, Camilla M	BKJ-Org.chem	BSc, 3rd yr	Universidad de Buenos Aires, Argentina
Myrstad, Marie	BKJ-E&A.chem	BSc, 3rd yr	University of New South Wales, Australia
Skjelbred, Kristin Marie	MTKJ-Phys.chem	MSc, 4th yr	University of California, San Diego, USA
Ringheim, Ingvild	MTKJ-Org.chem	MSc, 4th yr	Danmarks Tekniske Universitet, Denmark

Student exchange to NTNU, Department of Chemistry

Name	Institution
Agirrezabalaga Arraras, Mikel	University of the Basque, Spain
Baptist, Annelies	KU Leuven, Belgium
Barbarin Abarzuza, Iranzu	Univ. of Basque Country, San Sebastián, Spain
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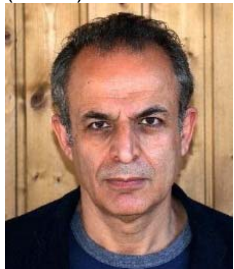
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Guest professors/researchers/lecturers

Marta Pokrzywnicka Faculty of Chemistry, University of Warsaw Project: "Monitoring of Marine Pollutants by Automated Remote System (POLAR)"	1.11.2012 – 1.3.2013
Barbara Nozière Institut de Recherches sur la Catalyse et l'Environnement de Lyon, France "Organic compounds and their chemical transformations in the earth atmosphere."	30.4.2013
Jon Pharoah Queen's-RMC fuel cell research centre, Queen's University, Kingston, Canada "Electrochemistry and the future of energy systems."	13.08.2013 - 15.09.2013
Mohamed Amedjkouh Fysikalsk organisk kjemi, Kjemisk Institutt, Universitetet i Oslo	26.09.2012 - 30.01.2013
Marie du Toit North-West University, Potchefstroom, South Africa.	09.09.2013 - 30.09.2013
Thorsten Hansen Department of Chemical Physics Lund University "2D Electronic Spectroscopy of Energy Transfer in Photosynthetic Antenna Complexes"	25.11.2013 - 29.11.2013
Professor Ana Martinez Universidad Nacional Autonoma de Mexico "Quantum chemistry for material sciences and birds."	5.12.2013 - 10.12.2013.
Kang Xue School of Resources and Materials Northeastern University at Qinhuangdao Kina.	26.06.2013 - 25.6.2014



The mountain king in the horizon

Annual Report for Department of Chemistry 2013



NTNU – Innovation and Creativity

The Norwegian University of Science and Technology (NTNU) in Trondheim represents academic eminence in technology and the natural sciences as well as in other academic disciplines ranging from the social sciences, the arts, medicine, architecture to fine arts. Cross-disciplinary cooperation results in ideas no one else has thought of, and creative solutions that change our daily lives.

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