

# MATEMAATIKA-LOODUSTEADUSKONNA KEEMIAINSTITUUDI TEADUS- JA ARENDUSTEGEVUSE AASTAARUANNE 2011

## 1. Instituudi struktuur

Instituudi direktor Mihkel Kaljurand

- Analüütilise keemia õppetool, Chair of Analytical Chemistry, Mihkel Kaljurand
- Anorgaanilise keemia õppetool, Chair of Inorganic Chemistry, Toomas Tamm
- Bioorgaanilise keemia õppetool, Chair of Bioorganic Chemistry, Nigulas Samel
- Biotehnoloogia õppetool, Chair of Biotechnology, Raivo Vilu
- Molekulaartehnoloogia õppetool, Chair of Molecular Technology, Mati Karelson
- Orgaanilise keemia õppetool, Chair of Organic Chemistry, Margus Lopp
- Keemilise analüüsi teadus- ja katselaboratoorium, Laboratory of Chemical Analysis

## 2. Instituudi teadus- ja arendustegevuse (edaspidi T&A) iseloomustus

*(NB! punktid 2.1- 2.6 täidab struktuuriüksus)*

*2.1.1 teadustöö kirjeldus (inglise keeles);*

*2.1.2 aruandeaastal saadud tähtsamad teadustulemused (inglise keeles).*

*2.2 Uurimisgrupi kuni 5 olulisemat publikatsiooni läinud aastal.)*

### **T725, Uued asümmeetrilise sünteesi strateegiad ja meetodid, teema juht Lopp Margus** **New strategies and methods of asymmetric synthesis**

The main goal of the project is to develop methods of the asymmetric synthesis by designing and elaborating of new chiral inducers (catalysts, including organocatalysts) and applying the new methods in the chemical synthesis of essential bioactive compounds. Within the project the mechanism/chemism of asymmetric transformations will be studied; a method for the synthesis of labeled compounds by asymmetric oxidation will be elaborated; possibilities of the synthesis of different chiral ligands and their complexes with metals (Ti, lanthanides etc) and the properties of the complexes will be investigated; the possibilities of the use of new chiral ligands in the asymmetric synthesis will be elucidated; in order to establish the structure/activity relationship of the new compounds (complexes), both, experimental and theoretical calculation will be used; general features of the interactions of substrate-chiral inducer in asymmetric oxidation and its enantioselectivity will be established; a method for the total chemical synthesis of 9,11-secosterols will be elaborated; a method for the synthesis of ribose analogs will be developed; new anti-cancer and anti virus nucleosides will be developed; a new method for N-monoalkylated (tertiary) or dialkylated (quaternary) amine derivatives will be developed; a method for cyclic amines starting from substituted aziridins will be developed; obtained compounds are used as chiral ligands and asymmetric organocatalysts.

#### **Tulemused 2011:**

##### **Publikatsioonid 2011:**

Noole, A.; Borissova, M.; Lopp, M.; Kanger, T. (2011). Enantioselective Organocatalytic Aza-Ene-Type Domino Reaction Leading to 1,4-Dihydropyridines. *Journal of Organic Chemistry*, 76(6), 1538 - 1545.

Gruselle, M.; Kanger, T.; Thouvenot, R.; Flambard, A.; Kriis, K.; Mikli, V.; Traksmäa, R.; Maaten, B.; Tõnsuaadu, K. (2011). Calcium Hydroxyapatites as Efficient Catalysts for the Michael CC Bond Formation. *ACS Catalysis*, 1729 - 1733.

Gundersen, L.-L.; Gorbitz, C.H.; Neier, L.; Roggen, H.; Tamm, T. (2011). Calculated tautomeric equilibria and X-ray structures of 2-substituted N-methoxy-9-methyl-9H-purin-6-amines. *Theoretical Chemistry Accounts*, 129(3-5), 349 - 358.

Aav, R.; Pehk, T.; Tamp, S.; Tamm, T.; Kudrjašova, M.; Parve, O.; Lopp, M. (2011). Theoretical prediction and assignment of vicinal <sup>1</sup>H-<sup>1</sup>H coupling constants of diastereomeric 3-alkoxy-6,7-epoxy-2-oxabicyclo[3.3.0]octanes. *MAGNETIC RESONANCE IN CHEMISTRY*, 49(2), 76 - 82.

Reile, I.; Paju, A.; Müürisepp, A.-M.; Pehk, T.; Lopp, M. (2011). Oxidation of cyclopentane-1,2-dione: a study with <sup>18</sup>O labeled reagents. *Tetrahedron*, 67(33), 5942 - 5948.

### **T023, Analüütilised lahutusmeetodid biomeditsiinis ja keskkonnakeemias. teema juht Kaljurand Mihkel**

#### **Analytical Separation Methods in Biomedicine and Environmental Chemistry**

The research aims at developing new methods of analytical separation to the characterization of various samples of biological origin. The research will focus on the following.

- 1) A search for new buffers for CE using mixtures of organic solvents and ionic liquids.
- 2) The investigation of potential extragents and development of methods for the determination of the composition and antioxidative ability of plant extracts.
- 3) The miniaturization of CE instruments aiming at developing portable analyzers to solve environmental problems in situ.
- 4) The production of nanopore materials, aerogels, to be used to separate various analytes by electrochromatography.

#### **Results:**

1. Portable analyser was tested successfully in the field experiments with genuine chemical warfare agents
2. Proof of a principle of the CE-ESI-MS ja CE-MALDI-MS off-line interfacing using digital and droplet microfluidics was demonstrated.
3. New aerogels were synthesized

#### **Publications:**

Palmre, V.; Lust, E.; Jänes, A.; Koel, M.; Peikolainen, A.-L.; Torop, J.; Johanson, U.; Aabloo, A. (2011). Electroactive polymer actuators with carbon aerogel electrodes. *Journal of Materials Chemistry*, 21, 2577 - 2583.

Kuban, P.; Seiman, A.; Makarõtševa, N.; Vaher, M.; Kaljurand, M. (2011). In situ determination of Sarin, Soman and VX nerve agents in various matrices by portable capillary electropherograph with contactless conductivity detection. *Journal of Chromatography A*, 1218(18), 2618 - 2625.

Helmja, K.; Vaher, M.; Kaljurand, M. (2011). Evaluation of the free radical scavenging capability of wheat extracts by capillary electrophoresis and multivariate curve resolution. *Electrophoresis*, 32(9), 1094 - 1100.

Seiman, A.; Vaher, M.; Kaljurand, M. (2011). Thermal marks as a signal processing aid for portable capillary electropherograph. *Electrophoresis*, 32(9), 1006 - 1014.

Peikolainen, A.-L.; Volobujeva, O.; Aav, R.; Uibu, M.; Koel, M. (2011). Organic acid catalyzed synthesis of 5-methylresorcinol based organic aerogels in acetonitrile. *Journal of Porous Materials*, 1 - 6.

### **T190, Toidu süsteemibioloogia ja füüsika, teema juht Vilu Raivo** **Food systems biology and physics**

The key subjects of the study were: lactic acid bacteria, probiotics and yeast; single cell model of microorganisms; growth space of microorganisms; peptides and bioactive compounds. The aim of the project was development of systems biology of microorganisms and food production processes using omics methods and mathematical modelling.

**Tulemused:**

Development multi-omics approach to study the growth efficiency and amino acid metabolism of bacteria.

**Publikatsioonid:**

Kriščiunaite, T.; Stulova, I.; Taivosalo, A.; Laht, T.-M.; Vilu, R. (2012). Composition and renneting properties of raw bulk milk in Estonia. *International Dairy Journal*, 23(1), 45 - 52.

Kabanova, N.; Stulova, I.; Vilu, R. (2012). Microcalorimetric study of the growth of bacterial colonies of *Lactococcus lactis* IL1403 in agar gels. *Food Microbiology*, 29(1), 67 - 79.

Valgepea, K.; Adamberg, K.; Vilu, R. (2011). Decrease of energy spilling in *Escherichia coli* continuous cultures with rising specific growth rate and carbon wasting. *BMC Systems Biology*, 5, 106

Lahtvee, P.-J.; Adamberg, K.; Arike, L.; Nahku, R.; Aller, K.; Vilu, R. (2011). Multi-omics approach to study the growth efficiency and amino acid metabolism in *Lactococcus lactis* at various specific growth rates. *Microbial Cell Factories*, 10(Article no.12), -

Kriščiunaite, T.; Stulova, I.; Kabanova, N.; Laht, T.-M.; Vilu, R. (2011). The effect of hydrogen peroxide on the growth of thermophilic lactic starter and acid gelation of UHT milk. *International Dairy Journal*, 21(4), 239 - 246.

**T133, Biokatalüütiline stereokeemiline süntees, teema juht Parve Omar**  
**Biocatalytic stereochemical synthesis.**

**Teadustöö kirjeldus:**

Lipase-catalysed reactions of polyhydroxy compounds have been investigated.

Methods of the chemoenzymatic synthesis of deoxy sugar esters as well as hydroxy acid conjugates have been elaborated.

Drastic change in catalytic performance of a lipase in methanolysis of esters depending on methanol content in reaction medium has been studied.

**Tähtsamad teadustulemused:**

Modelling of solvation of *Thermomyces lanuginosa* lipase using MD simulation combined with docking studies was found to rationalize the steered catalytic performance of this enzyme in methanolysis of 11-acetyl-prostaglandin E2. Chemoenzymatic methods of synthesis of deoxy sugar esters of amino acids were elaborated.

**2011 ilmunud tööd,:**

1. Villo, L.; Kreen, M.; Kudryashova, M.; Metsala, A.; Tamp, S.; Lille, Ü.; Pehk, T.; Parve, O. (2011). A Chemoenzymatic Synthesis of Deoxy Sugar Esters Involving Stereoselective Acetylation of Hemiacetals Catalyzed by CALB. *Journal of Molecular Catalysis B: Enzymatic*, 68(1), 44 - 51.

2. Villo, L.; Kreen, M.; Kudryashova, M.; Metsala, A.; Tamp, S.; Lille, Ü.; Pehk, T.; Parve, O. (2011). A chemoenzymatic synthesis of a deoxy sugar ester of N-Boc-protected L-tyrosine. In: John Whittall, Peter Sutton (Editors). *Practical Methods for Biocatalysis and Biotransformations* (1 - 6). USA, Canada, Euroopa, Austraalia, Aasia: Wiley-Blackwell [in press]

3. Aav, R.; Pehk, T.; Tamp, S.; Tamm, T.; Kudrjašova, M.; Parve, O.; Lopp, M. (2011). Theoretical prediction and assignment of vicinal 1H–1H coupling constants of diastereomeric 3-alkoxy-6,7-epoxy- 2-oxabicyclo[3.3.0]octanes. *MAGNETIC RESONANCE IN CHEMISTRY*, 49(2), 76 - 82.

4. Kaevand, T.; Kalda, J.; Kukk, V.; Öpik, A.; Lille, Ü. (2011). Correlation of the morphology and electrical conductivity in thin films of PEDT/PSS complex: an integrated meso-scale simulation study. *Molecular*

Simulation, 37(6), 495 - 502.

5. Villo, L.; Metsala, A.; Tamp, S.; Pehk, T.; Parve, O. (2011). A Synthesis of Deoxy Sugar Esters. Stereoselective Acetylation of Hemiacetals by CALB. *Biotrans* 2011; Itaalia, Giardini Naxos, 02.-05.10.2011.

## **T010, Bioaktiivsed lipiidid - metabolism, signaaliülekannet ja regulatsioon , teema juht Samel Nigulas Bioactive lipids - metabolism, signalling and regulation**

### **2.1.1. Description of research objectives**

Lipids are essential components of the cell membrane shown to play many dynamic roles in mediating and controlling a wide array of cellular activities including membrane structure, metabolic and gene regulation, protein structure and function, energy production, and signalling pathways. Lipid mediators have been intimately linked to the immune and inflammatory responses, cell proliferation and apoptosis, as well as shown to be major determinants in many pathologies, including diabetes, cancer, cardiovascular and neurodegenerative disorders. Lipid metabolizing enzymes and lipid-regulating and lipid-producing metabolic cascades have been targeted for drug development. The main goals of the research are: (i) elucidation of fundamental catalytic, metabolic and regulatory aspects of enzymes (cyclooxygenases, lipoxygenases and peroxidases) responsible for biosynthesis of lipid mediators, and (ii) study of regulatory mechanisms of lipoprotein metabolism by apolipoproteins and angiopoietins.

### **2.1.2. The most important finding**

Several recent studies reveal a link between lipoprotein/lipid metabolism and virus infections. It is demonstrated that cell surface glycans and members of the low density receptor family, both are well known to mediate binding and uptake of lipoproteins to cell, interact also with several viruses. Furthermore, lipases and apolipoproteins influence binding of viruses to cell surfaces. Even life-cycle of viral replication depends on cholesterol and fatty acid biosynthesis. In the current collaborative study the mechanisms that regulate the action of adenovirus 37 (Ad37) were investigated. It is demonstrated that adenovirus type 37 interacts with previously unknown sialic acid-containing cell surface molecules. Ad37 is a leading cause of epidemic keratoconjunctivitis a severe and highly contagious ocular disease. Glycan array screening and surface plasmon resonance experiments revealed that the receptor-recognizing knob domain of the virus fiber protein specifically binds a branched hexasaccharide that is present in the GD1a ganglioside. Soluble GD1a glycan and GD1a-binding antibodies efficiently prevented Ad37 virions from binding and infecting corneal cells. Unexpectedly, the receptor is constituted by one or more glycoproteins containing the GD1a glycan motif rather than the ganglioside itself, as shown by binding, infection and flow cytometry experiments. Surface plasmon resonance, molecular modeling, nuclear magnetic resonance and X-ray crystallography measurements indicate that the two terminal sialic acids dock into two of three previously established sialic acid-binding sites in the trimeric Ad37 knob. Surface plasmon resonance analysis shows that the knob-GD1a glycan interaction has high affinity. These observations form a basis for the design and development of sialic acid-containing antiviral drugs for topical treatment of epidemic keratoconjunctivitis. Nilsson et al., *Nature Medicine*, 2011, 105-109.

### **2.2. Main publications:**

Nilsson, E.C.; Storm, R.J.; Bauer, J.; Johansson, S.M.; Löökene, A.; Angström, J.; Hedenström, M.; Eriksson, T.L.; Frängsmyr, L.; Rinaldi, S.; Willison, H.J.; Domellöf, F.P.; Stehle, T.; Arnberg, N. (2011). The GD1a glycan is a cellular receptor for adenoviruses causing epidemic keratoconjunctivitis. *Nature Medicine*, 17 (1), 105 - 109.

Kobzar, G.; Mardla, V.; Samel, N. (2011). Short-term exposure of platelets to glucose impairs inhibition of platelet aggregation by cyclooxygenase inhibitors. *Platelets*, 22, 338 - 344.

**T031A, Uued arvutusmeetodid keerukate biomolekulide süsteemide kirjeldamiseks, teema juht Karelson Mati**  
**Modeling of biomedically and environmentally important systems using computational chemistry**

The subject of the research has been the computational study of detailed mechanisms of interactions of chemical compounds with the living organisms and environment. The research has been carried out by the development of new computational methods and the respective software. The novel methodological approaches include development of (1) ab initio quantum-chemical descriptors for molecules in external fields; (2) new quantum molecular dynamics based molecular docking techniques; (3) new algorithms for the search of optimum conformational structure of flexible molecules; and (4) implementation of advanced mathematical methods for the structure-activity relationships. The methodology developed is applicable for the description and prediction of (1) physicochemical properties; (2) pharmacodynamic and pharmacokinetic data; (3) antiviral activity of compounds; (4) activity of mimetics of neurotrophic factors; (5) structure and properties of peptide delivery vectors.

**Tähtsamad teadustulemused**

Numerous biologically important properties of chemical compounds including their toxicity, bioavailability, micelle formation ability, model properties related to drug intestinal absorption (Caco-2, PAMPA) and solubility were successfully modeled using the QSAR/QSPR approach. Successful models were also developed for the prediction of cell-penetrating peptides. The extension of the the methods to predict the antiviral and anti-b-amyloid activities carbon nanostructures, e.g. fullerenes is of particular interest.

**Olulisemad publikatsioonid 2011**

J.Kovacs, P. Kacsuk, A. Lomaka, Using a private desktop grid system for accelerating drug discovery, Future Generation Computer Systems the International Journal of Grid Computing and Escience, 27, 657-666 (2011).

A.R. Katritzky, I.B. Stoyanova-Slavova, K. Tamm, T. Tamm and M. Karelson, Application of the QSPR Approach to the Boiling Points of Azeotropes, J. Phys. Chem. A., 115, 3475-3479 (2011).

M. Karelson, D. Dobchev, Using artificial neural networks to predict cell-penetrating compounds, Expert Opinion in Drug Discovery, 6, 783-796 (2011).

---

**2.3** Loetelu struktuuriüksuse töötajate rahvusvahelistest tunnustustest.

**2.4** Loetelu struktuuriüksuse töötajatest, kes on välisakadeemiate või muude oluliste T&A-ga seotud välisorganisatsioonide liikmed.

**2.5** Aruandeaasta tähtsamad T&A finantseerimise allikad: sihtfinantseeritavad teemad (6), ETF grandid(10), välisprojektid (TAP6-3, VFP414, VA452, EU28912, VA433), siseriiklikud lepingud(12).

**2.6** Soovi korral lisada aruandeaastal saadud T&A-ga seotud tunnustusi (va punktis 2.3 toodud tunnustused), ülevaate teaduskorralduslikust tegevusest, teadlasmobiilsusest ning anda hinnang oma teadustulemustele.

**Tunnustusi:**

17.02.2011: Pikaajalise tulemusliku teadus- ja arendustöö eest määrati riigi teaduspreemia Ülo Lillele

23.-27. veebruarini 2011 toimub TTÜ keemiainstituudi korraldusel Rakveres rahvusvaheline talvekool kemomeetrias. Peakorraldajad Mihkel Koel, Mihkel Kaljurand ja Maria Borissova.

International Conference on Materials and Technologies for Green Chemistry. Tallinn 05.-09.09.2011. Peakorraldajad Mihkel Koel ja Maria Borissova.

07.12.2011 Valis Eesti Teaduste Akadeemia üldkogu keemia alal akadeemikuks orgaanilise keemia professori Margus Loppi.

## 2.7 Instituudi teadus- ja arendustegevuse teemade ja projektide nimetused (*Eesti Teadusinfosüsteemi, edaspidi ETIS, andmetel*)

- Haridus- ja Teadusministeerium

sihtfinantseeritavad teemad:

- T725, Uued asümmeetrilise sünteesi strateegiad ja meetodid, Lopp Margus
- T023, Analüütilised lahutusmeetodid biomeditsiinis ja keskkonnakeemias, Kaljurand Mihkel
- T190, Toidu süsteemibioloogia ja füüsika, Vilu Raivo
- T133, Biokatalüütiline stereokeemiline süntees, Parve Omar
- T010, Bioaktiivsed lipiidid - metabolism, signaaliülekanne ja regulatsioon, Samel Nigulas
- T031A, Uued arvutusmeetodid keerukate biomolekulide süsteemide kirjeldamiseks, Karelson Mati

baasfinantseerimise toetusfondist rahastatud projektid (sh TTÜ tippkeskused):

riiklikud programmid:

BF148 – M.Kaljurand – Massispektromeetri Q-Star Elite hoolduskulude osaline kompenseerimine.  
01.10.2010-01.08.2011

BF145 – Aivar Lõokene – Pinna plasmonite resonantsi seadme BIAcore hooldus ning kasutusvõimaluste laiendamine

- Teiste ministeeriumide poolt rahastatavad riiklikud programmid:

- Uurija-professori rahastamine:

Oleg Kulinkovich

- SA Eesti Teadusfond

grandid:

- ETF7135, Asümmeetriliste organokatalüütiliste reaktsiooniteede modelleerimine, Uudsema Merle
- ETF8250, Alküülimidiasoolium soolade kasutamine mass-spektromeetria liitsüsteemides, Borissova Maria
- ETF8276, 11R-lipoksügenaasi katalüütiliste omaduste modifitseerimine, Järving Ivar
- ETF7818, Fraktsioonide kogumine kapillaarelektroforeesis, Kaljurand Mihkel
- ETF8289, Efektiivsus organokatalüüsis, Kanger Tõnis
- ETF7636, Juustu mikrostruktuuri mõju biokeemilistele ja mikrobioloogilistele protsessidele juustu valmimise ajal, Laht Tiiu-Maie
- ETF8300, Angiopoietini sarnaste valkude 3 ja 4 molekulaarsed toimemehhanismid lipoproteiinide metabolismis, Lõokene Aivar
- ETF8255, Asümmeetriline induktsioon konformatsiooniliselt paindlikes süsteemides, Tamm Toomas
- ETF7941, Prostaglandiinide biosüntees punavetikates, Varvas Külliki
- ETF8698, Uute asümmeetriliste iminofosfatraanide süntees, analüüs ja rakendamine, Riina Aav

ühisgrandid välisriigiga:

järel doktorite grandid (SA ETF ja Mobilitas):

- MJD2, New MS-based approaches for studies of conformation and aggregation of amyloidogenic peptides, Gehenn Katja
- MJD105, Structure-reactivity relationships in reactions at atoms of the third period elements, Ploom Anu

tippteadlase grandid (Mobilitas):

- Ettevõtluse Arendamise SA

eeluuringud:

arendustoetused:

- SA Archimedeseaga sõlmitud lepingud  
infrastruktuur (nn „mini-infra“, „asutuse infra“):
  - AP023, Analüütilised lahutusmeetodid biomeditsiinis ja keskkonnakeemias, Kaljurand Mihkel
  - ÜLTAP63, Loodusteaduste Maja infrastruktuuri edasiarendus, Mihkel Koel

Eesti tippkeskused:

- TAR8103; TAR8103A, Keemilise bioloogia tippkeskus - Asümmeetriline süntees, Margus Lopp
- TAR8103B, Keemilise bioloogia tippkeskus - Nanotehnoloogilised süsteemid, Mati Karelson

riiklikud programmid:

- AR10130, Anaeroobsel kääritamisel põhinevate biogaasi energiatehnoloogiate biokeemiliste protsesside optimeerimine ning monitooringu ja juhtimismeetodite arendamine, Raivo Vilu, Mihkel Kaljurand
- AR11122, Piimhappebakterite süsteemioloogiline disain, Raivo Vilu, Mihkel Kaljurand

muud T&A lepingud:

- SA Keskkonnainvesteeringute Keskusega sõlmitud lepingud:
- Siseriiklikud lepingud:
  - Lep11120 (OÜ Eesti Keskkonnauuringute Keskus) – Tiina Randla – Kvaliteedi tagamise (QA – quality assurance) kontrolli aruande Eesti riikliku kasvuhoonegaaside 2012. aasta inventuuri ja inventuuriaruande kohta.
  - Lep10053, Reoveesette ja teiste biolagunevate jäätmete koos- ja eraldikäitlemine anaeroobse kääritamise teel Eestis ja digestaadile jäätmelõpu kriteeriumist lähtuvalt soovituslike kasutuskriteeriumide väljatöötamine, Vilu Raivo
  - Lep11018, Bakterite LGG ja La-5 vastupanuvõime määramine subletaalsele stressile kasutades microarray kiipide tehnikaid ning proteoomikat, Vilu Raivo
  - Lep11037, Üherakumudeli struktuuriparameetrite analüüsi kompuuteriseerimismeetodite väljatöötamine, Vilu Raivo
  - Lep11084, Juustupiima kvaliteet ja selle mõju pika valmimisajaga juustude valmistamisel ning farmipiima kvaliteedi seos sööda kvaliteedi hügieeningimustega piima tootmisel, Laht Tiiu-Maie
  - LMIN10119A, Energeetika ja põllumajanduse valdkondade Eesti riikliku kasvuhoonegaaside 2011. aasta inventuuri ja inventuuriaruande koostamine, Vilu Raivo
  - PRIA10029, Mittestandardse ja sekundaarse kalatoorme väärimise uuring. Vesiviljeluse kvaliteedi uuring, Vilu Raivo
  - LMIN11073, (Keskkonnaministeerium + KIK) – Inge Roos (MS soojustehnika instituut) ja Raivo Vilu – Energeetika ja põllumajanduse valdkondade Eesti riikliku kasvuhoonegaaside 2012 aasta inventuuri ja inventuuriaruande koostamine.
- EL Raamprogrammi projektid:
  - VFP414, Developing the research potential of Institute of Chemistry at Tallinn University of Technology, Estonia, Kaljurand Mihkel
  - TAP6-3, EU structural funds, üleülikooliline projekt) – projekti juht Mihkel Koel – Loodusteaduste maja infrastruktuuri edasiarendus
- Välisriiklikud lepingud:
  - VA452, Asymmetric threat environment analysis (through asymmetric engagement modelling, modelling of impacts on hearts and minds, and threat scenario generation from environmental factors, Idla Katrin
  - EU28912 – R.Vilu – Kolmemõõtmelise front-face fluorentsents-spektromeetria rakendamine. 2009-2011
  - VA433 – T.Kanger – Design of heterogeneous metal catalysts supported on apatite.2009-2011

**2.8** Strukturiüksuse töötajate poolt avaldatud sihtfinantseeritava teadusteema taotlemisel arvestatavad eelretsenseeritavad teaduspublikatsioonid (*ETIS klassifikaatori alusel 1.1, 1.2, 1.3, 2.1, 2.2, 3.1, 3.2, 3.3, 4.1 ja 5.1*).

### 1.1

Kaljurand, M.; Koel, M. (2011). Recent Advancements on Greening Analytical Separation. *Critical Reviews in Analytical Chemistry*, 41(1), 2 - 20.

Roggen, Heidi; Bohlin, Lars; Burman, Robert; Charnock, Colin; Felth, Jenny; Gorbitz, Carl Henrik; Larsson, Rolf; Tamm, Toomas; Gundersen, Lise-Lotte (2011). 2-Substituted agelasine analogs: Synthesis and biological activity, and structure and reactivity of synthetic intermediates. *Pure and Applied Chemistry*, 83(3), 645 - 653.

Villo, L.; Kreen, M.; Kudryashova, M.; Metsala, A.; Tamp, S.; Lille, Ü.; Pehk, T.; Parve, O. (2011). A Chemoenzymatic Synthesis of Deoxy Sugar Esters Involving Stereoselective Acetylation of Hemiacetals Catalyzed by CALB. *Journal of Molecular Catalysis B: Enzymatic*, 68(1), 44 - 51.

Gruselle, M.; Kanger, T.; Thouvenot, R.; Flambard, A.; Kriis, K.; Mikli, V.; Traksmaa, R.; Maaten, B.; Tõnsuaadu, K. (2011). Calcium Hydroxyapatites as Efficient Catalysts for the Michael CC Bond Formation. *ACS Catalysis*, 1729 - 1733.

Gundersen, L.-L.; Gorbitz, C.H.; Neier, L.; Roggen, H.; Tamm, T. (2011). Calculated tautomeric equilibria and X-ray structures of 2-substituted N-methoxy-9-methyl-9H-purin-6-amines. *Theoretical Chemistry Accounts*, 129(3-5), 349 - 358.

Kulp, M.; Bragina, O.; Kogerman, P.; Kaljurand, M. (2011). Capillary electrophoresis with led-induced native fluorescence detection for determination of isoquinoline alkaloids and their cytotoxicity in extracts of *Chelidonium majus* L. . *Journal of Chromatography A*, 1281(31), 5298 - 5304.

Vaher, M.; Koel, M.; Kazarjan, J.; Kaljurand, M. (2011). Capillary electrophoretic analysis of neutral carbohydrates using ionic liquids as background electrolytes. *Electrophoresis*, 32(9), 1068 - 1073.

Raal, A.; Kaur, H.; Orav, A.; Arak, E.; Kailas, T.; Müürisepp, M. (2011). Content and composition of essential oils in some Asteraceae species. *Proceedings of the Estonian Academy of Sciences*, 60(1), 55 - 63.

Kaevand, T.; Kalda, J.; Kukk, V.; Öpik, A.; Lille, Ü. (2011). Correlation of the morphology and electrical conductivity in thin films of PEDT/PSS complex: an integrated meso-scale simulation study. *Molecular Simulation*, 37(6), 495 - 502.

Valgepea, K.; Adamberg, K.; Vilu, R. (2011). Decrease of energy spilling in *Escherichia coli* continuous cultures with rising specific growth rate and carbon wasting. *BMC Systems Biology*, 5, 106

Koel, M.; Borissova, M.; Vaher, M.; Kaljurand, M. (2011). Developments in the application of Green Chemistry principles to food analysis. *AGRO FOOD INDUSTRY HI-TECH*, 22(5), 27 - 29.

Põldma, P.; Tõnutare, T.; Viitak, A.; Luik, A.; Moor, U. (2011). Effect of selenium treatment on mineral nutrition, bulb size, and antioxidant properties of garlic (*Allium sativum* L.). *Journal of Agricultural and Food Chemistry*, 59(10), 5498 - 5503.

Palmre, V.; Lust, E.; Jänes, A.; Koel, M.; Peikolainen, A.-L.; Torop, J.; Johanson, U.; Aabloo, A. (2011). Electroactive polymer actuators with carbon aerogel electrodes. *Journal of Materials Chemistry*, 21, 2577 - 2583.

Gorbatsova, J.; Borissova, M.; Kaljurand, M. (2011). Electrowetting-on-dielectric actuation of droplets with capillary electrophoretic zones for off-line mass spectrometric analysis. *Journal of Chromatography A*, xxx - xxx. [ilmumas]



- Noole, A.; Borissova, M.; Lopp, M.; Kanger, T. (2011). Enantioselective Organocatalytic Aza-Ene-Type Domino Reaction Leading to 1,4-Dihydropyridines. *Journal of Organic Chemistry*, 76(6), 1538 - 1545.
- Orav, A.; Arak, E.; Raal, A. (2011). Essential oil composition of *Coriandrum sativum* L. fruits from different countries. *Journal of Essential Oil Bearing Plants*, 14(1), 118 - 123.
- Orav, A.; Arak, E.; Boikova, T.; Raal, A. (2011). Essential oil in *Betula* spp. leaves naturally growing in Estonia. *Biochemical Systematics and Ecology*, 39(4-6), 744 - 748.
- Helmja, K.; Vaher, M.; Kaljurand, M. (2011). Evaluation of the free radical scavenging capability of wheat extracts by capillary electrophoresis and multivariate curve resolution. *Electrophoresis*, 32(9), 1094 - 1100.
- Kuban, P.; Seiman, A.; Kaljurand, M. (2011). Improving precision of manual hydrodynamic injection in capillary electrophoresis with contactless conductivity detection. *Journal of Chromatography A*, 1218(9), 1273 - 1280.
- Kuban, P.; Seiman, A.; Makarõtseva, N.; Vaher, M.; Kaljurand, M. (2011). In situ determination of nerve agents in various matrices by portable capillary electropherograph with contactless conductivity detection. *Journal of Chromatography A*, 1218(18), 2618 - 2625.
- Krabbi, K.; Uudelepp, M.-L.; Joost, K.; Zordania, R.; Õunap, K. (2011). Long-term complications in Estonian galactosemia patients with a less strict lactose-free diet and metabolic control. *Molecular Genetics and Metabolism*, 103(3), 249 - 253.
- Zekker, I.; Rikmann, E.; Tenno, T.; Menert, A.; Lemmiksoo, V.; Saluste, A.; Tenno, T.; Tomingas, M. (2011). Modification of nitrifying biofilm into nitritating one by combination of increased free ammonia concentrations, lowered HRT and dissolved oxygen concentration. *Journal of Environmental Sciences*, 23(7), 1113 - 1121.
- Lahtvee, P.-J.; Adamberg, K.; Arike, L.; Nahku, R.; Aller, K.; Vilu, R. (2011). Multi-omics approach to study the growth efficiency and amino acid metabolism in *Lactococcus lactis* at various specific growth rates. *Microbial Cell Factories*, 10(Article no.12), -
- Peikolainen, A.-L.; Volobujeva, O.; Aav, R.; Uibu, M.; Koel, M. (2011). Organic acid catalyzed synthesis of 5-methylresorcinol based organic aerogels in acetonitrile. *Journal of Porous Materials*, 1 - 6.
- Reile, I.; Paju, A.; Müürisepp, A.-M.; Pehk, T.; Lopp, M. (2011). Oxidation of cyclopentane-1,2-dione: a study with <sup>18</sup>O labeled reagents. *Tetrahedron*, 67(33), 5942 - 5948.
- Laars, M.; Ausmees, K.; Kudrjashova, M.; Kanger, T.; Werner, F. (2011). rac -2,2'-Bipiperidine-1,1'-dium dibromide. *Acta Crystallographica Section E: Structure Reports Online*, 67, o1324
- Werner, F.; Toon, L.; Aav, R. (2011). rac -8a'-Methyl-3',4',8',8a'-tetrahydro-2'H-spiro-[[1,3]dioxolane-2,1'-naphthalen]-6'(7'H)-one. *Acta Crystallographica Section E: Structure Reports Online*, E67, o2460
- Kobzar, G.; Mardla, V.; Samel, N. (2011). Short-term exposure of platelets to glucose impairs inhibition of platelet aggregation by cyclooxygenase inhibitors. *Platelets*, 22, 338 - 344.
- Ploom, A.; Tuulmets, A.; Järv, J. (2011). Structure-reactivity relationships in organosilicon chemistry revisited. *Central European Journal of Chemistry*, 9(5), 910 - 916.
- Ausmees, K.; Selyutina, A.; Kütt, K.; Lippur, K.; Pehk, T.; Lopp, M.; Žusinaite, E.; Merits, A.; Kanger, T. (2011). Synthesis and biological activity of bimorpholine and its carbanucleoside. *Nucleosides Nucleotides & Nucleic Acids*, 30(11), 897 - 907.

Kriščiunaite, T.; Stulova, I.; Kabanova, N.; Laht, T.-M.; Vilu, R. (2011). The effect of hydrogen peroxide on the growth of thermophilic lactic starter and acid gelation of UHT milk. *International Dairy Journal*, 21(4), 239 - 246.

Nilsson, E.C.; Storm, R.J.; Bauer, J.; Johansson, S.M.; Löökene, A.; Angström, J.; Hedenström, M.; Eriksson, T.L.; Frängsmyr, L.; Rinaldi, S.; Willison, H.J.; Domellöf, F.P.; Stehle, T.; Arnberg, N. (2011). The GD1a glycan is a cellular receptor for adenoviruses causing epidemic keratoconjunctivitis. *Nature Medicine*, 17(1), 105 - 109.

Aav, R.; Pehk, T.; Tamp, S.; Tamm, T.; Kudrjašova, M.; Parve, O.; Lopp, M. (2011). Theoretical prediction and assignment of vicinal 1H–1H coupling constants of diastereomeric 3-alkoxy-6,7-epoxy-2-oxabicyclo[3.3.0]octanes. *MAGNETIC RESONANCE IN CHEMISTRY*, 49(2), 76 - 82.

Seiman, A.; Vaher, M.; Kaljurand, M. (2011). Thermal marks as a signal processing aid for portable capillary electrophoresis. *Electrophoresis*, 32(9), 1006 - 1014.

Kovacs, J.; Kacsuk, P.; Lomaka, A. (2011). Using a private desktop grid system for accelerating drug discovery. *Future Generation Computer Systems*, 27(26), 657 - 666.

Karelson, M.; Dobchev, D. (2011). Using artificial neural networks to predict cell-penetrating compounds. *Expert Opinion on Drug Discovery*, 6(8), 783 - 796.

Helmja, K.; Vaher, M.; Püssa, T.; Orav, A.; Viitak, A.; Levandi, T.; Kaljurand, M. (2011). Variation in the composition of the essential oils, phenolic compounds and mineral elements of *Hypericum perforatum* L. growing in Estonia. *Natural Product Research*, 25(5), 496 - 510.

## 1.2

Timberg, L.; Koppel, K.; Kuldjärv, R.; Paalme, T. (2011). Rainbow trout composition and fatty acid content in Estonia. *Agronomy Research*, 9(S2), 495 - 500.

Stulova, I.; Kabanova, N.; Kriščiunaite, T.; Laht, T.-M.; Vilu, R. (2011). The effect of milk heat treatment on the growth characteristics of lactic acid bacteria. *Agronomy Research*, 9, 473 - 478.

## 1.3

### 2.1

### 2.2

### 3.1

Villo, L.; Kreen, M.; Kudryashova, M.; Metsala, A.; Tamp, S.; Lille, Ü.; Pehk, T.; Parve, O. (2011). A chemoenzymatic synthesis of a deoxy sugar ester of N-Boc-protected L-tyrosine. John Whittall, Peter Sutton (Toim.). *Practical Methods for Biocatalysis and Biotransformations* (1 - 6). USA, Canada, Euroopa, Austraalia, Aasia: Wiley-Blackwell [ilmumas]

Friedrich Kaasik, Janno Torop, Anna-Liisa Peikolainen, Mihkel Koel and Alvo Aabloo (2011). Carbon aerogel based electrode material for EAP actuators. *Proc. SPIE (79760O)*.SPIE

Karelson, M.; Koppel, I.A.; Leito, I.; Kaljurand, M.; Samel, N.; Lopp, M.; Pehk, T. (2011). Chemistry in Estonia- Review and Outlook. Engelbrecht, J. (Toim.). *Research in Estonia, Present and Future* (319 - 345). Tallinn: Estonian Academy of Sciences

Kaljurand, M.; Koel, M. (2011). Green Analytical Separation Methods. Miguel de la Guardia; Salvador Garrigues (Toim.). *Challenges in Green Analytical Chemistry* (168 - 198). Royal Society of Chemistry

## 3.2

Lepane, V. (2011). HPLC Fingerprints of Porewater Organic Compounds as Markers for Environmental Conditions. Stephen S. Young, Steven E. Silvern (Toim.). Environmental Change (1 - 18).INTECH [ilmumas]

Zekker, I.; Rikmann, E.; Tenno, T.; Saluste, A.; Lemmiksoo, V.; Menert, A.; Loorits, L.; Tenno, T. (2011). Achieving nitrification and anammox enrichment in single moving bed biofilm reactor treating reject water. In: AGRO 2011, 8th IWA International Symposium on Waste Management Problems in Agroindustries. Cesme, Izmir, Turkey, 22-24 June 2011. Proceedings: AGRO 2011, 8th IWA International Symposium on Waste Management Problems in Agroindustries. , 2011, 827 - 828.

Rikmann, E.; Zekker, I.; Tomingas, M.; Tenno, T.; Menert, A.; Loorits, L.; Tenno, T. (2011). Sulfate-reducing anaerobic ammonium oxidation as a potential treatment method for high nitrogen-content wastewater. In: AGRO 2011, 8th IWA International Symposium on Waste Management Problems in Agroindustries. Cesme, Izmir, Turkey, 22-24 June 2011. Proceedings: AGRO 2011, 8th IWA International Symposium on Waste Management Problems in Agroindustries. , 2011, 755 - 762.

3.3

4.1

5.1

**2.9** Struktuuriüksuses kaitstud doktoriväitekirjade loetelu (*NB! struktuuriüksus lisab struktuuriüksuse töötaja juhendamisel mujal kaitstud doktoriväitekirjade loetelu*)

**Tatjana Knjazeva**, keemiainstituut

Teema: *New Approaches in Capillary Electrophoresis for Separation and Study of Proteins*

(Kapillaarelektroforeesi uued lahendused valkude lahutamisel ja uurimisel)

Juhendaja: prof Mihkel Kaljurand

Kaitses: 17.03.2011

Omistatud kraad: filosoofiadoktor (keemia)

**Andrus Seiman**, keemiainstituut

Teema: *Point-of-Care Analyser Based on Capillary Electrophoresis* (Kapillaarelektroforeesil põhinev kaasaskantav analüsaator)

Juhendaja: prof Mihkel Kaljurand

Kaitses: 29.06.2011

Omistatud kraad: filosoofiadoktor (keemia)

**Monika Mortimer**, keemiainstituut

Teema: *Evaluation of the Biological Effects of Engineered Nanoparticles on Unicellular Pro- and Eukaryotic organisms* (Sünteesiliste nanoosakeste bioloogiliste efektide hindamine üherakulistel pro- ja eukarüootsetel organismidel)

Juhendaja: prof Margus Lopp

Kaasjuhendaja: juhtivteadur Anne Kahru

Kaitses: 16.08.2011

Omistatud kraad: filosoofiadoktor (keemia)

**Natalja Makarõtševa**, keemiainstituut

Teema: *Analysis of Organic Species in Sediments and Soil by High Performance Separation Methods* (Orgaaniliste ainete analüüs sette ja mulla proovides kõrgefektiivsete lahutusmeetodite abil)

Juhendaja: dotsent Viia Lepane

Kaitses: 23.08.2011

Omistatud kraad: filosoofiadoktor (keemia)

**Kersti Tepp**, keemiainstituut

Teema: *Molecular System Bioenergetics of Cardiac Cells: Quantitative Analysis of Structure Function Relationship* (Molekulaarne süsteemibioenergeetika: südameraku struktuuri ja funktsiooni vaheliste suhete kvantitatiivne analüüs)

Juhendaja: prof Raivo Vilu

Kaasjuhendaja: juhtivteadur Valdur Saks

Kaitses: 7.10.2011

Omistatud kraad: filosoofiadoktor (keemia)

**Anna-Liisa Peikolainen**, keemiainstituut

Teema: *Organic Aerogels Based on 5-Methylresorcinol* (Orgaanilised aerogeelid 5-metüülresortsinoolist)

Juhendaja: juhtivteadur Mihkel Koel

Kaitses: 10.10.2011

Omistatud kraad: filosoofiadoktor (keemia)

**Jelena Gorbatšova**, keemiainstituut

Teema: *Development of Methods for CE analysis of Plant Phenolics and Vitamins* (KE meetodite väljatöötamine taimsete fenoolsete ühendite ja vitamiinide analüüsiks)

Juhendaja: prof Mihkel Kaljurand

Kaitses: 21.12.2011

Omistatud kraad: filosoofiadoktor (keemia)

## 2.10 Struktuuriüksuses järel doktorina T&A-s osalenud isikute loetelu (*ETIS-e kaudu esitatud taotluste alusel*)

MJD2, New MS-based approaches for studies of conformation and aggregation of amyloidogenic peptides,

**Gehenn Katja**

MJD105, Structure-reactivity relationships in reactions at atoms of the third period elements, **Ploom Anu**

## 2.11 Struktuuriüksuses loodud tööstusomandi loetelu

### **US2011152346A1**

Use of oligonucleotides with modified bases in hybridization of nucleic acids

Taotlus esitatud: 14.02.2011

Autorid: Mati Karelson, Erkki Truve, Allan Olsper, Cecilia Sarmiento, Mart Saarma

Omanik: Balti Tehnoloogiaarenduse AS

Instituudid: YK, YT

### **EE05449B1**

(2-Hüdroksü-3-okso-tsöklopent-1-enüül)-äädikhappe estrid ja meetod nendest ainetest (-)-R- ja (+)-S-homosidrunhappe gamma-laktooni ja vastavate (-)-R- ja (+)-S homosidrunhappe soolade valmistamiseks

Patent välja antud: 15.08.2011

Autorid: Margus Lopp, Anne Paju, Margus Eek, Marit Laos, Tõnis Pehk, Raissa Jäälaid

Omanikud: TTÜ, AS Cambrex Tallinn, AS VTAK

Instituut: YK

### **EE05457B1**

4'-arüül-2',3'-dideoksünukleosiidi analoogid

Patent välja antud: 15.08.2011

Autorid: Margus Lopp, Anne Paju, Artur Jõgi, Kaarel Siirde, Raissa Jäälaid, Tõnis Pehk

Omanikud: TTÜ, AS Cambrex Tallinn, AS VTAK

Instituut: YK

### **EP2156374B1**

A method for manufacturing of a smart packaging material

Patent välja antud: 05.10.2011

Autorid: Mati Karelson, Kaupo Karelson, Jaan Leis, Neinar Seli  
Omanik: Raidenil OÜ  
Instituut: YK

### **3. Struktuuriüksuse infrastruktuuri uuendamise loetelu**

- Suruõhu jahutussüsteem, 331,12.01.2011,3 070 €
- Spektrofotomeeter UV-Mini-1240,24.01.2011,2 575 €
- CD-spektromeeter TENSOR 27,9.05.2011,96 985 €
- Vedelik-kromatograafia analüüs,30.05.2011,483 788 €
- Metaani potentsiaali mõõtesüs-,1.06.2011,28 182 €
- OxiTop komplekt 1000 ml,13.07.2011,4 900 €
- OxiTop komplekt 250 ml,13.07.2011,4 827 €
- Peristaltiliste pumpade kompl.,11.08.2011,3 979 €
- MilliGas counter MGC-1 kompl.,26.08.2011,4 696 €
- Tõmbekapp Kojair 1800, 264,23.09.2011,10 692 €