MATEMAATIKA-LOODUSTEADUSKOND
KEEMIAINSTITUUT
TEADUS- JA ARENDUSTEGEVUSE AASTAARUANNE 2012

1. Instituudi struktuur

Keemiainstituut, Department of Chemistry
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 struktuuriüksuse koosseisu kuuluvate uurimisgruppide

2.1.1 teadustöö kirjeldus *(inglise keeles*);

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

2.2 uurimisgrupi kuni 5 olulisemat publikatsiooni

T060, Katalüütilise asümmeetrilise sünteesi ja stereokeemilise analüüsi meetodid ja rakendused, teema juht **Lopp Margus**
Methods and applications of catalytic asymmetric synthesis and stereochemical analysis.

BalticumOrganikumSyntheticum BOS 2012 in Tallinn. Margus Lopp, Head of the Local Organizing Committee.

International conference on Organic Synthesis BOS 2012 (BalticumOrganicumSyntheticum) June 1.juulist-July in Tallinn.Participants 350 scientists from 27 countries.One of the main plenary speaker Nobel Prize winner Professor Akira Suzuki from Japan.

BalticumOrganikumSyntheticum BOS 2012 Round Table *Bioactive compounds as the targets for organic synthesis.*Organizer Margus Lopp.

Teadustöö kirjeldus

The goal is to create and develop new methods of asymmetric organic synthesis by designing, preparing and introducing new chiral inducers and by finding new asymmetric transformations. The project is formally divided in three parts: new asymmetric reactions, computational design and analysis and synthesis of bioactive compounds. These parts are tightly linked and support each other. Asymmetric catalytic reactions and stereodirected cascade reactions of compounds with multiple prosterogenic centers creating stereoselectively multiple stereocenters simultaneously will be investigated. Computational modeling develops a robust and user-friendly method for the analysis of VCD spectra and supports understanding of properties and reaction mechanisms of the

compounds. The rationally designed nucleoside analogues, dopamine receptor modulators and cucurbiturils will be synthesized and their biological and other properties will be investigated.

Tulemused:

Research was carried out in two main directions: asymmetric organocatalysis and synthesis of biologically active compounds.

- A new cascade reaction leading to spirooxindoles bearing adjacent quaternary-tertiary stereocenters starting from 3-chlorooxinoles was found and developed. The synthesized compounds are used as building blocks in alkaloid synthesis and, in many cases, as starting materials in medicinal chemistry.
- A neworganocatalytic Michael addition of malonates to symmetric unsaturated 1,4-diketones catalyzed by thiourea and squaramide derivatives with *Cinchona* alkaloids afforded the formation of a new C–C bond in high yields (up to 98%) and enantiomeric purities (up to 93%).
- A new organocatalytic reaction of 1,2-diketones as nucleofiles afforded chiral enantiomeric 3-substituted 1,2-cyclopentanediones, which are valuable starting compounds in bioactive compound synthesis.
- New 3-aza and 3-oxabicyclo[3.2.0]heptane derivatives were synthesized via a general diastereoselctive three-component triple cascade reaction. The obtained compounds demonstrated bigger binding affinity at D2L and D3 dopamine receptors compared to D1 binding sites.
- Attempts to develop of the convenient methods for sulphur-containing nucleoside analogues continued. Several intermediate compounds were biologically tested.

Tähtsamad publikatsioonid 2012:

Noole, A.; Järving, I.; Werner, F.; Lopp, M.; Malkov, A.; Kanger, T. Organocatalytic Asymmetric Synthesis of 3-Chloroindoles Bearing Adjecent Quaterinary Centers. *Org.Lett*., **2012**, 14(18), 4922-4925.

Ausmees, K.; Kriis, K.; Pehk, T.; Noole, A.;.; Werner, F.; Järving, I., Lopp, M.; Kanger, T. Diastereoselective Multicomponent Cascade Reaction leading to {3.2.0] Heterobicyclic Compounds. *J.Org. Chem*., **2012**, 77(23), 10681-10687.

Reile, Indrek; Paju, Anne; Kanger, Tonis, Järving, Ivar; Margus, Lopp. Cyclopentane-1,2-dione bis(tert-butyldimethylsilyl) enol ether in asymmetric organocatalytic Mukaiyama-Michael reactions. *Tetrahedron Lett.,* **2012**, *53*, 1476-1478.

Reinart-Okubeni, R.;Ausmees, K.; Kriis, K.; Werner, F.; Rinken A.; Kanger, T. Chemoenzymaticsynthesis and evaluation of 3-azabicyclo[3.2.0]heptane derivativesasdopaminergicligands.*Eur. J. Med. Chem.*,55,255-261.

Zari, Sergei, Kudrjashova, Marina, Öeren, Mario; Järving, Ivar; Tamm, Toomas, Lopp, Margus; Kanger, Tõnis. Organocatalytic asymmetric addition of malonates to unsaturated 1,4-diketones. *Beilstein Journal of Organic Chemistry,* **2012**, *8*, 1452-1457.

Osaleti Bioloogilise Keemia Tippkeskuses (TAR803A) ja Biotehnoloogia programmi projektis

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

Analytical Separation Methods in Biomedicine and Environmetal 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.

Tulemused:
1) The paper microzone-based green analytical chemistry methods for determining the quality of wines was developed.
2) A new tool for ionic analysis of exhaled breath condensate- capillary electrophoresis was proposed
3) Electrowetting on dielectric actuation of droplets with capillary electrophoretic zones for MALDI mass spectrometric analysis was developed
4) Theory of green analytical chemistry was developed.

Tähtsamad publikatsioonid 2012:
1. Gorbatsova, J., Borissova, M., &Kaljurand, M. (2012). Electrowetting-on-dielectric actuation of droplets with capillary electrophoretic zones for off-line mass spectrometric analysis. *Journal of Chromatography A, 1234*, 9-15.
2. Koel, M., &Kaljurand, M. (2012). Benign design in analytical chemistry. *Critical Reviews in Analytical Chemistry, 42*(2), 192-195.
3. Kubáň, P., Kobrin, E., &Kaljurand, M. (2012). Capillary electrophoresis - A new tool for ionic analysis of exhaled breath condensate. *Journal of Chromatography A, 1267*, 239-245. Retrieved from
4. Holzweber, M., Lungwitz, R., Doerfler, D., Spange, S., Koel, M., Hutter, H., &Linert, W. (2013). Mutual Lewis acid-base interactions of cations and anions in ionic liquids. *Chemistry - A European Journal, 19*(1), 288-293.
5. Laheäär, A., Peikolainen, A., Koel, M., Jänes, A., & Lust, E. (2012). Comparison of carbon aerogel and carbide-derived carbon as electrode materials for non-aqueous supercapacitors with high performance. *Journal of Solid State Electrochemistry, 16*(8), 2717-2722.

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 of multi-omics approach to study the growth efficiency and amino acid metabolism of bacteria, development of microcalorimetric methods for the study of lactic acid bacteria in milk and milk gels.

Tähtsamad publikatsioonid 2012:

Arike, L.; Valgepea, K.; Peil, L.; Nahku, R.; Adamberg, K.; Vilu, R. (2012). Comparison and applications of label-free absolute proteome quantification methods on Escherichia coli. *Journal of Proteomics*, 75(17), 5437 - 5448.

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.

Adamberg, K.; Seiman, A.; Vilu, R. (2012). Increased Biomass Yield of Lactococcus lactis by Reduced Overconsumption of Amino Acids and Increased Catalytic Activities of Enzymes. *PLoS ONE*, 7(10), e48223

Pitk, P.; Kaparaju, P.; Vilu, R. (2012). Methane potential of sterilized solid slaughterhouse wastes. *Bioresource Technology*, 116, 42-46.

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.

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

Teadustöö kirjeldus:
Lipase-catalysed reactions of polyhydroxy compounds – among others diols and tetrols have been in the focus.
Chemoenzymatic methods for the synthesis of hydroxy acid conjugates using linking via glycolic acid spacer have been elaborated.
Modeling of some diols forming associates in their racematic and enantiopure form in different medium.

Tähtsamad teadustulemused:
Computational methods have shown that some diols can form different associates depending on their enantiomeric purity and media.
A simple procedure for linking chiral alcohol and hydroxycarboxylic acid via glycolic acid has been described. The high diastereomeric purity (>99.8%) of the conjugates with remote stereocenters has been determined by NMR spectroscopy.
Chemoenzymatic separation method for γ-lactone enantiomers from racemic mixture has been studied.
Lipase-catalyzed resolution has been used for obtaining enantiopure diols and tetrols from their racemic mixtures also in preparative scale.
Synthesis of enantiopure halohydrines from several diols has been described.

Tähtsamad publikatsioonid 2012:
Villo, L.; Kreen, M.; Kudryashova, M.; Metsala, A.; Tamp, S.; Lille, Ü.; Pehk, T.; Parve, O. (2012). 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 2 (335 - 339). USA, Canada, Euroopa, Austraalia, Aasia: Wiley-Blackwell

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

Descrription of research objectives

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.

The most important finding

Eek, P., Järving, R., Järving, I., Gilbert, N. C., Newcomer, M. E., Samel, N. (2012) Structure of a Calcium-dependent 11*R*-Lipoxygenase Suggests a Mechanism for Ca^{2+} Regulation. *Journal of Biological Chemistry*, 287, 22377 - 22386.

Study of the crystal structure of 11*R*-lipoxygenase in collaboration with researchers from Louisiana State University revealed that the active site of this enzyme forms a closed T-shaped channel with two potential entrances. Also, a strongly conserved π-cation bridge between the regulatory domain of the enzyme and the active site in the catalytic domain was detected. By the hypothesis of authors, during calcium binding to the regulatory domain the conformational changes are communicated to the catalytic domain via this bridge. The mouth of the active site opens and the enzyme becomes active. The proposed model of activation gives new insights into better understanding of regulation and specificity of lipoxygenases including human 5-LOX.

Tähtsamad publikatsioonid 2012:

Järving, R.; Lõokene, A.; Kurg, R.; Siimon, L.; Järving, I.; Samel, N. (2012). Activation of 11R-lipoxygenase is fully Ca(2+)-dependent and controlled by the phospholipid composition of the target membrane. ***Biochemistry***, 51(15), 3310 - 3320.

Robal, T.; Larsson, M.; Martin, M.; Olivecrona, G.; Lookene, A. (2012). Fatty Acids Bind Tightly to the N-terminal Domain of Angiopoietin-like Protein 4 and Modulate its Interaction with Lipoprotein Lipase. ***Journal of Biological Chemistry***, 287(35), 29739 - 29752.

Kukk, K.; Järving, R.; Samel, N. (2012). Purification and characterization of the recombinant human prostaglandin H synthase-2 expresssed in Pichia pastoris. ***Protein Expression and Purification***, 83(2), 182 -189.

Nilsson, S.K.; Anderson, F.; Ericsson, M.; Larsson, M.; Makoveichuk, E.; Lookene, A.; Heeren, J; Olivecrona, G. (2012). Triacylglycerol-rich lipoproteins protect lipoprotein lipase from inactivation by ANGPTL3 and ANGPTL4. ***Biochimica et Biophysica Acta - Molecular and Cell Biology of Lipids***, 1821(10), 1370 - 1378.

Eek, P.; Järving, R.; Järving, I.; Gilbert, N. C.; Newcomer, M. E.; Samel, N. (2012). Structure of a Calcium-dependent 11R-Lipoxygenase Suggests a Mechanism for Ca2+ Regulation. ***Journal of Biological Chemistry***, 287(26), 22377 - 22386.

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

A novel computational technology based on fragmentation of the chemical compounds has been used for the fast and efficient prediction of activities of prospective protease inhibitors of the hepatitis C virus. The studies spanned over a discovery cycle from the theoretical prediction of new HCV NS3 protease inhibitors to the first cytotoxicity experimental tests of the best candidates. The measured cytotoxicity of the compounds indicated that at least two candidates would be suitable further development of drugs. It was also discovered that extended molecular connectivity encoded by the Kier–Hall second order valence connectivity index provides an excellent correlation with ion mobility spectroscopy (IMS) cross-sections of tripeptides.

Olulisemad publikatsioonid 2012

Karelson, M.; Dobchev, D.A.; Karelson, G.; Tamm, T.; Tämm, K.; Nikonov, A.; Mutso, M.; Merits, A. (2012). Fragment-based development of HCV protease inhibitors for the treatment of hepatitis C. *Current Computer-Aided Drug Design*, 8(1), 55 - 61.

Oliferenko, A.A.; Tian, F.F.; Karelson, M. ; Katritzky, A.R. (2012). Prediction of peptide IMS cross sections from extended molecular connectivity. *International Journal of Mass Spectrometry*, 314, 1-5.

2.3 Loetelu struktuuriüksuse töötajate rahvusvahelistest tunnustustustest.

NATO teadus- ja tehnoloogiaorganisatsiooni teadussaavutuste auhind TTÜ molekulaartehnoloogia õppetooli teaduritele Katrin Idlale ja Marek Strandbergile, tegevuse eest NATO RTO Süsteemide ja kontseptsioonide integreerimise töörühmas.

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 (12), riiklikud programmid (4), välisprojektid (VFP414, VA452, VA433), siseriiklikud lepingud (8), SA Archimedese lepingud (3) ja tippkeskused (2).

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.

*TTÜ 2011. aasta teadlaseks valiti **Mihkel Kaljurand**, analüütilise keemia professor

*TTÜ 2011. aasta teadusartiklina toodi esile loodus-, täppis- ja terviseteaduste valdkonnas orgaanilise keemia õppetooli teadlaste publikatsioon: **Artur Noole, Maria Borissova, Margus Lopp, Tõnis Kanger** „Enantioselective Organocatalytic Aza-Ene-Type Domino Reaction Leading to 1,4-Dihydropyridines“. Journal of Organic Chemistry, 2011, 76, 6, 1538–1545. Artikkel publitseeriti orgaanilise keemia valdkonnas kõige enam viidatavas ajakirjas – *The Journal of Organic Chemistry*. Väärib märkimist, et artikkel publitseeriti esiletõstetuna (*featured article*). Igas ajakirjanumbris on mõned artiklid (tavaliselt 2-3), mis toimetaja valikul esile tõstetakse. Valiku tegemisel on olulisemateks kriteeriumiteks artikli teaduslik kvaliteet, üldine huvipakkuvus ja tähtsus.

*Septembrist 2012 sai matemaatika-loodusteaduskonna õppeprodekaaniks prof **Toomas Tamm**

*Eesti Vabariigi aastapreemia kandidaadiks keemia ja molekulaarbioloogia valdkonnas esitati matemaatika-loodusteaduskonna keemiainstituudi vanemteadur Aivar Lõokene uurimistöö „Lipoproteiinide metabolismi regulatsioonimehhanismid“ eest

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

- Haridus- ja Teadusministeerium

– sihtfinantseeritavad teemad:

T023, Analüütilised lahutusmeetodid biomeditsiinis ja keskkonnakeemias, Kaljurand Mihkel (2008 – 2013)

T191, Toidu süsteemibioloogia ja füüsika, Vilu Raivo (2008 – 2013)

T133, Biokatalüütiline stereokeemiline süntees, Parve Omar (2008 – 2013)

T010, Bioaktiivsed lipiidid - metabolism, signaaliülekanne ja regulatsioon , Samel Nigulas (2008 – 2013)

T031A, Uued arvutusmeetodid keerukate biomolekulide süsteemide kirjeldamiseks, Karelson Mati (2009 – 2014)

T060, Katalüütilise asümmeetriline sünteesi ja stereokeemilise analüüsi meetodid ja rakendused, Lopp Margus (2012 – 2014)

– baasfinantseerimise toetusfondist rahastatud projektid (sh TTÜ tippkeskused):

B14, Vanemteadur Aivar Lõokese uurimisgrupi toetamine, (2012 – 2012)

– riiklikud programmid:

- Teiste ministeeriumide poolt rahastatavad riiklikud programmid:
- Uurija-professori rahastamine:
- SA Eesti Teadusfond/Eesti Teadusagentuur

– grandid:

ETF8698, Uute asümmeetriliste iminofosfatraanide süntees, analüüs ja rakendamine, Aav Riina (2011 – 2014)

ETF8250, Alküülimidasoolium soolade kasutamine mass-spektromeetria liitsüsteemides, Borissova Maria (2010 – 2012)

ETF8276 , 11R-lipoksügenaasi katalüütiliste omaduste modifitseerimine, Järving Ivar (2010 – 2013)

ETF9106, Mikrotsoon paberlehtedel baseeruvate rohelise analüütilise keemia meetodite arendamine, Kaljurand Mihkel (2012 – 2015)

ETF8289, Efektiivsus organokatalüüsis, Kanger Tõnis (2010 – 2013)

ETF8986, Hybriidne mikrokapillaarelektroforeesi systeem kiireks lahutamiseks, Kuban Petr (2012 - 31.05.2012)

ETF8300, Angiopoietiini sarnaste valkude 3 ja 4 molekulaarsed toimemehhanismid lipoproteiinide metabolismis, Lõokene Aivar (2010 – 2013)

ETF9410, Rasvappedioksügenaaside ekspressioon ja oksülipiinide süntees korallis stressitingimustes, Samel Nigulas (2012 – 2015)

ETF8255, Asümmeetriline induktsioon konformatsiooniliselt paindlikes süsteemides, Tamm Toomas (2010 – 2013)

ETF7135, Asümmeetriliste organokatalüütiliste reaktsiooniteede modelleerimine, Uudsemaa Merle (2007 – 2012)

ETF79 , Prostaglandiinide biosüntees punavetikates, Varvas Külliki (2009 – 2012)

ETF9192, Oomikameetodite arendamine bakterite kvantitatiivsete süsteemibioloogiliste uuringute jaoks, Vilu Raivo (2012 – 2015)

– ühisgrandid välisriigiga:
– järeldoktorite grandid (SA ETF ja Mobilitas):

MJD105, Ploom Anu,Structure-reactivity relationships in reactions at atoms of the third period elements (1.09.2010 - 30.11.2014)

– tippteadlase grandid (Mobilitas):

- Ettevõtluse Arendamise SA

– eeluuringud:
– arendustoetused:

- SA Archimedesega sõlmitud lepingud

– infrastruktuur (nn „mini-infra“, „asutuse infra“):

AP023A, Analüütilised lahutusmeetodid biomeditsiinis ja keskkonnakeemias, Kaljurand Mihkel (1.01.2012 - 31.12.2013)

AP060, Katalüütilise asümmeetriline sünteesi ja stereokeemilise analüüsi meetodid ja rakendused, Lopp Margus (1.01.2012 - 31.12.2013)

ÜLTAP63, Loodusteaduste Maja infrastruktuuri edasiarendus, Mihkel Koel (1.01.2010 - 19.04.2012)

– Eesti tippkeskused:

TAR8103, Keemilise bioloogia tippkeskus - Asümmeetriline süntees, Margus Lopp (7.07.2008 - 31.08.2015)
TAR8103B, Keemilise bioloogia tippkeskus - Nanotehnoloogilised süsteemid, Mati Karelson (7.07.2008 - 31.08.2015)

– riiklikud programmid:

AR11122, Biotehnoloogia,Piimhappebakterite süsteembioloogiline disain, Raivo Vilu (1.09.2011 - 31.08.2014)

AR10130, Energiatehnoloogia,Anaeroobsel kääritamisel põhinevate biogaasi energiatehnoloogiate biokeemiliste protsesside optimeerimine ning monitooringu ja juhtimissüsteemi arendus, Raivo Vilu (1.04.2010 - 31.08.2015)

AR12124, materjalitehnoloogia, Electroactive nanoporous carbon composite films technology, Mihkel Koel (1.07.2012 - 31.12.2014)

AR12129B, materjalitehnoloogia, High-tech anti-wear coatings based in nanoparticles/ionic liquid combination for metal and engineering industries (TRIBOFILM), Mihkel Koel (1.08.2012 - 31.12.2014)

– muud T&A lepingud:

- SA Keskkonnainvesteeringute Keskusega sõlmitud lepingud:

LMIN11073A – Energeetika ja põllumajanduse valdkondade Eesti riikliku kasvuhoonegaaside 2012 aasta inventuuri ja inventuuriaruande koostamine, Inge Roos (MS soojustehnika instituut) ja Raivo Vilu (07.09.2010- 31.10.2012)

- Siseriiklikud lepingud:

Lep10053, Reoveesette ja teiste biolagunevate jäätmete koos- ja eraldikäitlemine anaeroobse kääritamise teel Eestis ja digestaadile jäätmelõpu kriteeriumist lähtuvalt soovituslike kasutuskriteeriumide väljatöötamine, Vilu Raivo (26.04.2010 - 28.03.2012)

Lep11084, Juustupiima kvaliteet ja selle mõju pika valmimisajaga juustude valmistamisel ning farmipiima kvaliteedi seos sööda kvaliteedi hügieenitingimustega piima tootmisel, Laht Tiiu-Maie (1.09.2011 - 31.08.2014)

Lep11120, Kvaliteedi tagamise (QA) kontrolli aruanne Eesti riikliku kasvuhoonegaaside 2012. aasta inventuuri ja inventuuriaruande kohta, Randla Tiina (9.12.2011 - 8.02.2012)

Lep12123 – Põllumajanduse valdkonna Eesti riikliku kasvuhoonegaaside (KHG) heitkoguste 2013. aasta inventuuri ja inventuuriaruande koostamine, Olga Gavrilova (21.08.2012 -31.10.2013)

Lep12122 – Energia- ja rohemajanduse seire, Mihkel Kaljurand (01.07.2012-30.09.2012)

Lep12091 – Näitus-konverentsi „Soldier technology 2012" külastamine ja ülevaate koostamine kavandatavast kaitse- ja julgeolekutehnoloogiate arengusuunast. Mihkel Kaljurand (-14.06.2012).

LEP12008 – Eelkatsed uudsete mudelkütustega (sisend taastuvtoormel kütuselisandite tehnoloogia hankimiseks ja juurutamiseks, Katrin Idla (21.12.2011-21.03.2012)

Lep12051 – Lihatööstuses tekkivate biojäätmete kasutusvõimalused anaeroobse kääritamise protsessis, Raivo Vilu (Peep Pitk) (01.03.2012-26.04.2012)

- EL Raamprogrammi projektid:

VFP414, TTÜ keemiainstituudi teaduspotentsiaali arendamine, Kaljurand, Mihkel (1.02.2009 - 31.01.2012)

- Välisriiklikud lepingud:

VA452, Asümmeetriliste ohtude hindamine ja analüüs, Idla Katrin (9.03.2010 - 9.09.2012)
VA433 – Design of heterogeneous metal catalysts supported on apatite, T.Kanger (2009-2014)

2.8 Struktuuriüksuse töötajate poolt avaldatud 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

Välbe, Raul; Mäeorg, Uno; Lõhmus, Ants; Reedo, Valter; Koel, Mihkel; Krumme, Andres; Kessler, Vadim; Hoop, Andres; Romanov, Alexey E. (2012). A novel route of synthesis of sodium hexafluorosilicate two component cluster crystals using BF4- containing ionic liquids. Journal of Crystal Growth, 361, 51 - 56.

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

Indrek Reile, keemiainstituut
Teema: *3-Alkylcyclopentane-1,2-Diones in Asymmetric Oxidation and Alkylation Reactions* (3-alküültsüklopentaan-1,2-dioonid asümmeetrilistes oksüdeerimis- ja alküleerimis-reaktsioonides)
Juhendaja: prof Margus Lopp
Kaitses: 15.03.2012
Omistatud kraad: filosoofiadoktor (keemia)

Külliki Krabbi, keemiainstituut
Teema: *Biochemical Diagnosis of Classical Galactosemia and Mucopolysaccharidoses in Estonia* (Klassikalise galaktoseemia ja mukopolüsahharidooside biokeemiline diagnostika Eestis)
Juhendajad: vanemteadur Tiiu-Maie Laht ja prof Katrin Õunap
Kaitses: 6.06.2012
Omistatud kraad: filosoofiadoktor (keemia)

Olga Gavrilova, keemiainstituut
Teema: *Application and Elaboration of Accounting Approaches for Sustainable Development* (Jätkusuutliku arengu arvestusmeetodite arendamine ja rakendamine)
Juhendaja: prof Raivo Vilu
Kaitses: 26.10.2012
Omistatud kraad: filosoofiadoktor (keemia)

Ranno Nahku, keemiainstituut
Teema: *Validation of Critical Factors for the Quantitative Characterization of Bacterial Physiology in Accelerostat Cultures* (Kriitiliste faktorite valideerimine bakterite füsioloogia uurimiseks akselerostaatsetes kultiveerimiseksperimentides)
Juhendajad: vanemteadur Kaarel Adamberg ja prof Raivo Vilu
Kaitses: 7.11.2012
Omistatud kraad: filosoofiadoktor (keemia)

Petri-Jaan Lahtvee, keemiainstituut
Teema: *Quantitative Omics-Level Analysis of Growth Rate Dependent Energy Metabolism in*

Lactococcus Lactis (Kvantitatiivsetel oomika-meetoditel põhinev kasvuerikiirusest sõltuv Lactococcus lactis-e energiametabolismi analüüs)
Juhendaja: prof Raivo Vilu, vanemteadur Kaarel Adamberg
Kaitses: 12.11.2012
Omistatud kraad: filosoofiadoktor (keemia)

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

Ploom Anu,Structure-reactivity relationships in reactions at atoms of the third period elements (1.09.2010 - 30.11.2014)

2.11 Struktuuriüksuses loodud tööstusomandi loetelu

EE20120008
Bioreaktorite süsteem ja meetod mikroorganismide füsioloogilise seisundi kloonimiseks
Taotlus esitatud: 16.05.2012
Autorid: Sten Erm, Raivo Vilu, Kaarel Adamberg
Omanikud: TTÜ, AS Toidu- ja Fermentatsioonitehnoloogia Arenduskeskus

EE05510B1
Orgaanilise aerogeeli valmistamise meetod
Patent välja antud: 15.02.2012
Autorid: Anna-liisa Peikolainen, Fernando Peréz-Caballero, Mihkel Koel
Omanik: TTÜ

US8148568
Esters of (2-Hydroxy-3-Oxo-Cyclopent-1-Enyl) Acetic Acid and their use for preparing (-)-R-Homocitric Acid Gamma-Lactone, (+)-S-Homocitric Acid Gamma-Lactone and the corresponding (-)-R-Homocitric Acid and (+)-S-Homocitric Acid Salts
Patent välja antud: 03.04.2012
Autorid: Margus Lopp, Anne Paju, Marit Laos, Tõnis Pehk, Raissa Jäälaid, Margus Eek.
Omanikud: TTÜ, VTAK, AS Cambrex Tallinn

3. Struktuuriüksuse infrastruktuuri uuendamise loetelu *(summa eurodes)*

PV007280, gaasikromatograaf, 17.01.2012 (30 668,09)

PV007437, CHNS elementanalüsaator, 331, 14.08.2012 (56 500,00)

PV007438, Kromatograaf-massispektromeeter, 27.08.2012 (59 087,86)

PV007491, GaussView 5 Site Lic x86_64/LX, 30.11.2012 (2 440,00)