Univerza *v Ljubljani*
Fakulteta *za kemijo in kemijsko tehnologijo*

POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2010

Univerza *v Ljubljani*
Fakulteta *za kemijo in kemijsko tehnologijo*

POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2010

ANNUAL REPORT 2010

Ljubljana, 2011

KAZALO

UVODNA BESEDA

Poročilo o izobraževalni in raziskovalni dejavnosti v letu 2010, ki ga prebirate, opisuje delo in dosežke sodelavcev Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani (FKKT UL) v letu, ki ga je v Sloveniji zaznamovala gospodarska kriza, na fakulteti pa se težave gospodarstva še niso močno odrazile. Uspeli smo zadržati in na nekaterih področjih tudi izboljšati kakovost našega pedagoškega in raziskovalnega dela. V uvodu bi rad povzel nekaj pomembnih dejstev z glavnih področij našega delovanja.

V letu 2010 je prva generacija bolonjskih študentov končala prvi letnik. Izkazalo se je, kar smo tudi pričakovali, da je bolonjski študij zahtevnejši od starega, predvsem zaradi večjega števila izpitov in ostrejših pogojev za napredovanje v višji letnik. To se je odrazilo v nekoliko zmanjšani prehodnosti v drugi letnik. S problemom smo se spoprijeli že pred koncem študijskega leta s spodbujanjem predmetnega tutorstva in dodatnimi govorilnimi urami pedagoških delavcev pri nekaterih predmetih. Da smo se težave lotili na pravi način dokazuje naslednja generacija študentov, ki ima že precej manj težav kot predhodna. V letu 2010 smo tudi pripravili vlogo za mednarodno akreditacijo »Eurobachelor in Chemistry« študijskega programa Kemija pri ECTNA (European Chemistry Thematic Network Association), ki je obrodila sadove v letu 2011 in prinesla prvo mednarodno akreditacijo kateremu od naravoslovnih študijskih programov v Sloveniji.

Na področju raziskovalnega dela je bilo leto 2010 posebej ugodno, saj smo na razpisu ARRS uspeli pridobiti sredstva, ki so skupaj z lastnim vložkom omogočila nakup 500 MHz NMR spektrometra ter s sovlaganjem inštitutov in industrije še vrstičnega elektronskega mikroskopa z izvorom elektronov na poljsko emisijo. Ob koncu leta smo z dodatno dodeljenimi sredstvi ARRS kupili še tekočinski kromatograf z masnim spektrometrom z analizatorjem na čas preleta ionov. Tako je bil postavljen temelj za oblikovanje Infrastrukturnega centra UL FKKT, ki naj bi združeval veliko raziskovalno opremo, omogočal njeno prosto dostopnost in olajšal njeno vzdrževanje ter pokrivanje materialnih stroškov delovanja.

Kot že v preteklih letih, je bilo tudi v letu 2010 vloženega veliko truda v priprave na gradnjo nove stavbe. Skoraj do konca je bil zgrajen most čez Glinščico, za dokončanje pa bomo potrebovali novega izvajalca, ker je šel CPM v stečaj. Veliko delo je bilo opravljeno na pripravi vloge za odobritev evropskih sredstev za gradnjo, saj je predvideni znesek tako velik, da mora projekt odobriti neposredno Evropska komisija. V letu 2010 je bil narejen bistven napredek, saj je vlogo potrdila evropska agencija JASPERS, kar predstavlja najbolj bistven korak do končne potrditve.

Vsem sodelavcem Fakultete za kemijo in kemijsko tehnologijo se iskreno zahvaljujem za vloženi trud in uspešno delo, ki sta pripeljala do dobrih rezultatov in potrdila visoko kakovost delovanja fakultete. Prepričan sem, da bomo s skupnim zavzetim delom tudi v prihodnje skrbeli za uspešnost in ugled FKKT UL.

Prof. dr. Anton Meden
Dekan

FOREWORD

The following report presents educational and research achievements of the Faculty of Chemistry and Chemical Technology, University of Ljubljana, for the period of 2010. In general, the year 2010 was marked by economic crisis, but fortunately, we have not felt all its negative effects yet. We managed to keep up with good work and in some areas even improved the quality of our teaching and research. Let me just mention some main areas of our activities and highlight some important facts:

In 2010, the first generation of students completed their first year of studies under Bologna programmes. As expected, Bologna system proved to be more difficult and demanding for students than previous study programmes, mainly due to more exams and stricter conditions for advancing into subsequent year. As we had anticipated, less students managed to complete their study obligations to enrol in the second year. In our attempts to tackle this problem we introduced tutorship for main subjects and professors offered additional contact hours for students. This strategy seemed to be a correct approach since the new generation of students this year are facing fewer problems than their colleagues last year.

In 2010 we applied for international accreditation to obtain "Eurobachelor in Chemistry" for our Chemistry study programme with ECTNA (European Chemistry Thematic Network Association). In 2011 we won accreditation, and are proud to say that this was the first international accreditation awarded to a science faculty in Slovenia.

For our researchers, 2010 was a lucky year in particular: we applied for the funds with Slovenian Research Agency (ARRS) and managed to receive funding, which, combined with our own investments, allowed us to purchase a new 500 MHz NMR Spectrometer. In addition to that, and with financial participation of some institutes and industries, we managed to buy a Field emission scanning electron microscope. At the end of the year we received some additional funds from ARRS and purchased a Liquid chromatograph coupled to time-of-flight mass spectrometer. With this new equipment we have formed a sound basis for setting up a new Infrastructural centre of UL FKKT in the future, a centre in which large research equipment would be located in one place, available to all researchers, while maintenance and material costs would be easier to cover.

Like in previous years, numerous attempts have been made towards bringing our construction project closer to the end. Part of the project has almost been finished by building a bridge across the Glinščica river, however, we will need to find a new building contractor to finish the works because the contractor CPM was declared bankrupt. We have put a lot of efforts into collecting documentation for applying for European funds to build our new faculty. The estimated amount is so high that the project will need approval from the European Commission directly. However, an important step forward has been made when the project was approved by the European agency JASPERS, which is a crucial step before final financial approval.

I wish to express my sincere appreciation to all my associates at the Faculty of Chemistry and Chemical Technology for all the fine work they have done, for the good results they have produced, and thus reconfirmed high quality of our work. I believe that in future too, with enthusiasm and hard work of all, we will manage to achieve more positive results and retain high reputation of our Faculty.

Prof. Dr. Anton Meden
The Dean

Modernega življenja si brez sodobne kemije ne moremo niti zamisliti, pa čeprav se tega v vsakdanjem življenju ne zavedamo. Brez kemije ni moderne biologije, ni farmacevtskih ved, ni razumevanja v medicini Brez kemijskega inženirstva ne bi bilo racionalne proizvodnje neštetih izdelkov, za katere se nam zdi samoumevno, da nam pripadajo.

V naših krajih ima študij in raziskovalno delo na področju kemijskih ved dolgo tradicijo. Prvi začetki segajo že v sedemnajsto stoletje, o začetku rednega študija na področju kemijskih ved pa lahko govorimo od leta 1919, ko je bila ustanovljena ljubljanska Univerza.

Kot zanimivost velja poudariti, da je bil prvi doktorat ljubljanske univerze podeljen leta 1920 iz kemije Anki Mayer.

POSLANSTVO FAKULTETE

Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani:

- Goji temeljno, aplikativno in razvojno raziskovanje na področjih kemije, biokemije, kemijskega inženirstva, požarne varnosti ter varnosti pri delu.
- Pri tem si prizadeva, da bi dosegla odličnost in najvišjo kakovost.
- Na osnovi lastnega raziskovanja ter lastnih in tujih raziskovalnih dosežkov izobražuje vodilne znanstvenike in strokovnjake, ki so usposobljeni za vodenje trajnostnega razvoja, ob upoštevanju izročila evropskega razsvetljenstva in humanizma ter ob upoštevanju človekovih pravic. Pri tem spodbuja interdisciplinarni in multidisciplinarni študij.
- Izmenjuje svoje dosežke na področju znanosti in umetnosti z drugimi univerzami in znanstvenoraziskovalnimi ustanovami. Tako prispeva svoj delež v svetovno zakladnico znanja in iz nje prenaša znanje v slovenski prostor. Sodeluje z gospodarstvom in s tem pospešuje uporabo svojih raziskovalnih in izobraževalnih dosežkov ter prispeva k družbenemu razvoju.
- Fakulteta utrjuje akademsko skupnost profesorjev, raziskovalcev, študentov in drugih sodelavcev ter si prizadeva za svojo uveljavitev doma in v svetu.
- Svoje raziskovanje, izobraževanje, javno delovanje in razmerja med člani utemeljuje na načelih profesionalne odličnosti, oziroma zagotavljanja čim višje kakovosti ter akademske svobode sodelavcev in študentov, s poudarkom na ustvarjalni svobodi.

MISSION STATEMENT

The FKKT members individually and collectively strive to:

- *Perform basic, applied and development research in the fields of chemistry, biochemistry, chemical engineering, fire safety and safety at work, endeavouring to achieve excellence and top quality of their work.*
- *Promote high quality teaching standards based on the results of their own research and other research groups to generate scientists and professionals who will be able to support and manage sustainable development based on the principles of European enlightenment and humanism and human rights. The faculty promotes interdisciplinary and multidisciplinary studies.*
- *Exchange the results with other universities and scientific research institutions in the fields of sciences and arts, in order to contribute to the world depository of knowledge as well as drawing on its knowledge.*
- *Develop cooperation with Slovenian industry and foster the application of its research and educational achievements, thus contributing its share to the general social development.*
- *Endeavour to establish itself nation wise and abroad by creating an academic community of teachers, researchers, students and other associates.*
- *Ground their research and educational activities, as well as public relations among its members on the principles of professional excellence, and promote highest quality and creative freedom by allowing academic freedom to the faculty staff and students.*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST

Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani (UL FKKT) izvaja Nacionalni program visokega šolstva in Nacionalni raziskovalni in razvojni program na področju kemije, biokemije, kemijskega izobraževanja, kemijskega inženirstva, polimernih ter keramičnih materialov in tehnologij, uporabne kemije, kemijske tehnologije, tehniške varnosti in požarne varnosti. Obenem opravlja na njihovih mejnih področjih izobraževalno, znanstveno-raziskovalno, razvojno, svetovalno ter druge s tem povezane dejavnosti. Osnovne izobraževalne in raziskovalne enote so katedre.

IZOBRAŽEVALNA DEJAVNOST

UL FKKT je v študijskem letu 2009/2010 pričela z izvajanjem prvostopenjskih univerzitetnih študijskih programov:

- Kemija
- Biokemija
- Kemijsko inženirstvo
- Tehniška varnost

prvostopenjskega visokošolskega strokovnega študijskega programa

- Kemijska tehnologija

ter prenovljenega doktorskega programa (tretjestopenjski univerzitetni študijski program)

- Kemijske znanosti

V letu 2010 se je na UL FKKT izvajalo tudi pet predbolonjskih dodiplomskih študijskih programov:

- univerzitetni program Kemija s smerema
    - Kemija
    - Kemijsko izobraževanje
- univerzitetni program Biokemija
- univerzitetni program Kemijsko inženirstvo
- visokošolski strokovni program Kemijska tehnologija s smerema

  - Kemijska tehnologija
  - Uporabna kemija
- visokošolski strokovni program Varstvo pri delu in požarno varstvo

FKKT je izvajala tudi tri podiplomske študijske programe:
- Kemija
- Kemijsko inženirstvo
- Kemijska tehnologija

Poleg tega pa je UL FKKT sodelovala z drugimi fakultetami pri izvajanju naslednjih podiplomskih študijskih programov:
- Biomedicina za področje Biokemije in molekularne biologije
- Bioznanosti
- Materiali
- Varstvo okolja

Pri Svetu Republike Slovenije za visoko šolstvo so akreditirani tudi drugostopenjski magistrski študijski programi Kemija, Biokemija, Kemijsko inženirstvo, Tehniška varnost in Kemijsko izobraževanje. V študijskem letu 2010/2011 smo zaradi velikega zanimanja diplomantov visokošolskega strokovnega študija Varstva pri delu in požarnega varstva pričeli z izvajanjem drugostopenjskega magistrskega študijskega programa Tehniška varnost.

Za izvedbo študijskih programov skrbi 35 rednih profesorjev, 14 izrednih profesorjev, 6 docentov, 1 višji predavatelj, 1 predavatelj, 53 asistentov, 3 strokovni sodelavci, 2 učitelja veščin ter 26 strokovnih delavcev.

RAZISKOVALNA DEJAVNOST

Na Fakulteti za kemijo in kemijsko tehnologijo so raziskave pomemben del dejavnosti učiteljev in sodelavcev. Temeljne raziskave omogočajo spremljanje svetovnega razvoja in napredka na področju naravoslovja in tehnologije, razvojne in uporabne raziskave pa predstavljajo stik med fakulteto in gospodarstvom.

Znanstveno in raziskovalno delo na fakulteti je bistveno povezano s podiplomskim izobraževanjem, saj lahko fakulteta le tako zagotavlja mednarodno konkurenčen študij. Raziskave v kemiji pokrivajo aktualna področja iz anorganske in organske sinteze, študij anorganskih in organskih spojin, analizne kemije, fizikalne in biofizikalne kemije, različnih vej biokemije, kot so encimatika, molekularna genetika in genski inženiring. Kemijsko inženirske raziskave pokrivajo področja razvoja procesov za anorganske in organske produkte ter materiale, reakcijskega inženirstva, transportnih pojavov, reologije, bioinženirstva, ekološkega inženirstva idr.

Raziskovalno delo je povezano tudi z industrijsko problematiko, predvsem za kemijsko, farmacevtsko, živilsko industrijo in biotehnologijo, gradbeništvo, varovanje okolja idr.

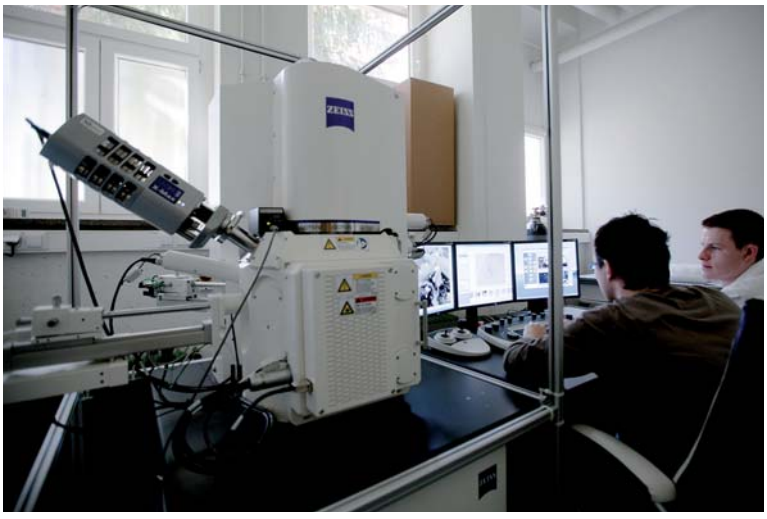
Pomembne so tudi interdisciplinarne raziskave, ki se izvajajo med različnimi fakultetami slovenskih univerz in drugimi slovenskimi znanstvenimi institucijami, ter mednarodne povezave v sklopu mednarodnih projektov in sodelovanja s tujimi univerzami ali raziskovalnimi laboratoriji.

DELOVANJE NMR INFRASTRUKTURNEGA CENTRA NA UL FKKT V LETU 2010

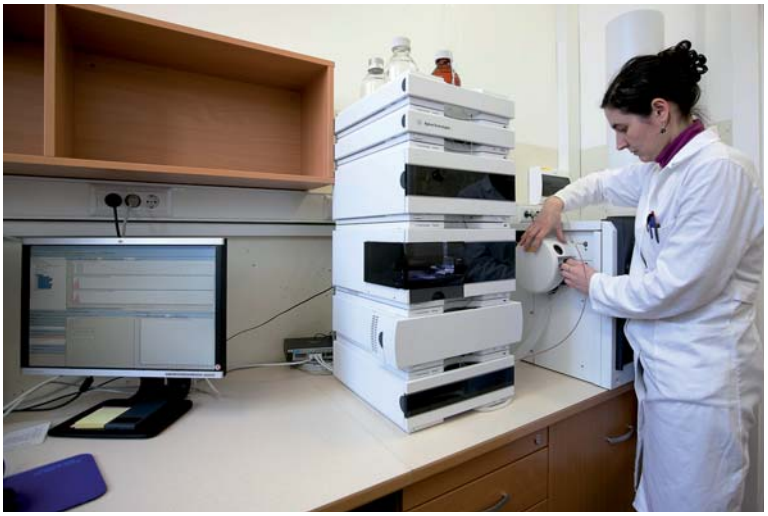
NMR infrastrukturni center na UL FKKT deluje v sklopu Mreže raziskovalnih infrastrukturnih centrov Univerze v Ljubljani (MRIC UL). Materialne stroške delovanja opreme sofinancira ARRS.

BRUKER AVANCE III
500 MHz NMR spektrometer

Kot je bilo načrtovano, je bil v letu 2010 BRUKER DPX 300 NMR inštrument NMR infrastrukturnega centra UL FKKT na razpolago uporabnikom 24 ur na dan, 7 dni v tednu, 52 tednov v letu. Od skupno 8760 ur so meritve tekle 7223 ur oziroma 82,5 % vsega razpoložljivega časa. Edina večja težava, ki je zahtevala večji poseg od rednega tedenskega vzdrževanja je bila okvara kompresorja, ki smo ga zamenjali z novim. Vsak ponedeljek je bil čas rezerviran za redno tedensko vzdrževanje in kalibriranje inštrumenta ter za zunanje uporabnike. Rezervacija inštrumentalnega časa poteka preko interneta (http://alkimist.fkkt.uni-lj.si). Informacije, povezane z delovanjem inštrumenta in razpored uporabe nočnih terminov objavljamo na domači strani NMR centra UL FKKT (http://nmr-slave.fkkt.uni-lj.si). Inštrument so pri raziskovalnem in pedagoškem delu uporabljali sodelavci UL Fakultete za kemijo in kemijsko tehnologijo in UL Fakultete za farmacijo. Rezultati raziskav, pri katerih so bile izvedene meritve z opremo centra v letu 2010, so



Vrstični elektronski mikroskop na poljsko emisijo Zeiss ULTRA plus



Agilent 6224 Accurate Mass TOF LC/MS sistem

bili objavljeni v 54 izvirnih znanstvenih člankih, v šestih preglednih znanstvenih člankih, desetih vabljenih predavanjih, štirih objavljenih znanstvenih prispevkih na konferencah, 85 prispevkih na konferencah z objavljenimi povzetki, 5 končnih poročilih o rezultatih raziskav ter 5 patentnih prijavah in 1 patentu. Oprema infrastrukturnega centra je bila uporabljena tudi pri raziskavah v sklopu 8 doktorskih disertacij ter dveh magistrskih in 28 diplomskih del.

V letu 2009 je bilo v okviru razpisa ARRS za sofinanciranje nakupa raziskovalne opreme (14. paket) odobreno sofinanciranje nakupa dveh NMR inštrumentov (400 in 500 MHz). Po zapletih in ponovljenem javnem razpisu smo v letu 2010 investicijo uspešno zaključili. 400 MHz NMR inštrument je nameščen v laboratoriju Fakultete za farmacijo in 500 MHz v laboratoriju Fakultete za kemijo in kemijsko tehnologijo. V decembru 2010 je potekalo usposabljanje uporabnikov na obeh inštrumentih, od 1. 1. 2011 pa sta oba inštrumenta v redni uporabi.

V teku je preoblikovnje NMR infrastrukturnega centra na UL FKKT v Infrastrukturni center UL FKKT (IC UL FKKT), v sklopu katerega bomo skrbeli za nabavo, vzdrževanje in uporabo velike raziskovalne opreme. V sklop delovanja IC bomo poleg NMR inštrumentov, vključili tudi elektronski mikroskop, ki je bil na FKKT kupljen s sofinanciranjem ARRS (14. paket). Dodatna namenska sredstva za opremo (infrastrukturno dejavnost), ki jih je ARRS konec leta 2009 namenila UL, smo na UL FKKT namenili za nakup analitskega inštrumenta LC-MS, ki omogoča določanje kromatografske čistote in natančne molekulske mase spojin. Meritve bomo izvajali v obliki servisa. Usluge bodo dostopne vsem raziskovalcem z UL in ostalih raziskovalnih ustanov. IC bo organiziran v obliki tematskih enot: enota za NMR, enota za MS, enota za EM. V bodočnosti bomo delovanje tudi ostale velike opreme organzirali pod okriljem IC, kar bo pripomoglo k ekonomičnejšemu delovanju, olajšanemu dostopu do inštrumentalnega časa in zmanjševanju podvajanja inštrumentalnih kapacitet.

MEDNARODNO SODELOVANJE

Mednarodno sodelovanje na Fakulteti za kemijo in kemijsko tehnologijo poteka tako na izobraževalnem kot na raziskovalnem področju. Na izobraževalnem področju se preko programa EU Vseživljenjsko učenje – Erasmus izvajajo izmenjave študentov na dodiplomskem in podiplomskem študiju. Program ponuja sofinanciranje izmenjav študentov za študij in prakso, učiteljev in administrativnega osebja.

V letu 2010 je bilo na izmenjavi v tujini, za študij in prakso, 18 naših študentov, iz tujine pa smo imeli na izmenjavi štiri študente. En naš učitelj se je udeležil izmenjave za predavanja v tujini in en učitelj iz tujine je gostoval pri nas.

V okviru Evropske Unije poteka tudi program za izmenjavo študentov Erasmus Mundus Basileus, ki omogoča izmenjave študentov v JV Evropo in iz nje. V okviru tega programa sta bila v letu 2010 pri nas na izmenjavi dva doktorska študenta iz Srbije.

Na raziskovalnem področju poteka sodelovanje na številnih dvostranskih projektih. V letu 2010 je Fakulteta za kemijo in kemijsko tehnologijo sodelovala pri 15 bilateralnih projektih z 12 državami. Na področju raziskovalnega dela na projektih COST sodeluje fakulteta na štirih projektih.

V okviru projektov Evropske Unije VŽU poteka, v letu 2010, raziskovalni projekt Leonardo da Vinci – prenos inovacij.

Na mednarodnem področju potekajo še druga sodelovanja z univerzami v ZDA, Braziliji, Avstriji, Srbiji, Bosni in Hercegovini in Makedoniji.

MEDNARODNA TEMATSKA KONFERENCA IMPLEMENTATION OF MICROREACTOR TECHNOLOGY INTO BIOTECHNOLOGY, IMTB 2010, NA FKKT

Na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani je 29. in 30. septembra 2010 potekala mednarodna tematska konferenca z naslovom **Vpeljava mikroreaktorske tehnologije v biotehnologijo** (*Implementation of Microreactor Technology into Biotechnology, IMTB 2010*).

Podobno kot je v prejšnjem stoletju mikroelektronika pomenila preobrat za informacijsko tehnologijo, predstavlja v tem stoletju mikroreaktorska tehnologija prelomnico in pomemben dejavnik razvoja na številnih področjih, od proizvodnje gorivnih celic, farmacevtske in kemijske industrije, do medicinske tehnologije, biotehnologije in okoljevarstva. Narava v številnih procesih že tisočletja uporablja prednosti mikrometrskega nivoja, saj so žive celice v bistvu biokemijski mikroreaktorji, večcelične oblike življenja pa izkoriščajo koncept povečanja šte-

V dveh dneh konference se je zvrstilo 24 vabljenih predavanj, ki so jih izvedli profesorji ter mlajši raziskovalci s številnih evropskih univerz ter nekaterih drugih znanstveno-raziskovalnih institucij. Sekcijo z naslovom »Modeliranje in integracija bioprocesov z zaključnimi procesi v mikrostrukturiranih napravah« sta vodila prof. dr. Želimir Kurtanjek in prof. dr. Bruno Zelić z Univerze v Zagrebu

vila (angl. numbering-up) v množici različic. Za razliko od narave sta znanost in tehnologija šele pred kratkim začeli izkoriščati pojave na mikro nivoju za praktično uporabo.

Konferenca IMTB 2010 je bila prva prireditev pri nas, ki je bila namenjena predstavitvi področja mikroreaktorske tehnologije s poudarkom na možnosti njene uporabe v biotehnologiji tako širši strokovni javnosti, sodelavcem kemijske, farmacevtske in drugih industrijskih panog, kot tudi študentom in mladim raziskovalcem s področja (bio)kemijskega inženirstva, biotehnologije, elektro in strojnega inženirstva, kemije, biologije, medicine idr.

Ob otvoritvi konference je udeležence poleg koordinatorice dogodka, doc. dr. Polone Žnidaršič Plazl s Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani ter prof. dr. Bruna Zelića z Univerze v Zagrebu nagovorila še prorektorica Univerze v Ljubljani, prof. dr. Julijana Kristl, v imenu gostiteljske fakultete pa je zbrane pozdravil tudi dekan FKKT UL, prof. dr. Anton Meden. V dveh dneh se je zvrstilo 24 predavanj, ki so jih izvedli profesorji ter mlajši raziskovalci s številnih univerz ter nekaterih drugih znanstveno-raziskovalnih institucij. Vabljeni predavatelji so bili s Fakultete za kemijo in kemijsko tehnologijo, Fakultete za strojništvo, Fakultete za elektrotehniko in Medicinske fakultete Univerze v Ljubljani, z Instituta Jožef Stefan, s Fakultete za kemijsko inženirstvo in tehnologijo in Prehrambeno biotehnološke fakultete Univerze v Zagrebu ter z Univerze v Southamptonu, Univerze v Padovi, Danske tehniške univerze, Tehniške univerze v Lizboni, Tehniške univerze v Gradcu in Tehniške univerze v Braunschweigu. Predavatelji so predstavili dosežke s področja izdelave mikrostrukturiranih naprav in njihove uporabe v biotehnologiji (encimski mikroreaktorji, mikrobioreaktorji za gojenje celic), miniaturizacije analitskih sistemov ter modeliranja in integracije bioprocesov z zaključnimi procesi v mikrostrukturiranih napravah. Prispevki predavateljev so zbrani tudi na zgoščenki, izdani ob tem dogodku.

Na konferenci je sodelovalo skoraj 100 udeležencev iz 11 držav, med katerimi je bilo največ dodiplomskih in podiplomskih študentov Univerze v Ljubljani ter raziskovalcev z institutov in industrije. Za vabljene udeležence prireditve je bil na Ljubljanskem gradu organiziran družabni dogodek, kjer je gostom večer obogatil slovenski glasbenik Vlado Kreslin, tujim predavateljem pa smo v okviru zavoda Turizem Ljubljana omogočili ogled znamenitosti našega mesta.

Na osnovi številnih razprav in tudi neformalnih pogovorov so se oblikovale številne ideje za nove raziskave in sodelovanja, tako v okviru dvostranskih kot tudi širših evropskih povezav. Glede na zelo pozitivne ocene udeležencev naj bi tovrstna konferenca, ki je prvič združevala različne strokovnjake s področja izdelovanja, razvoja in uporabe mikroreaktorske tehnologije iz vse Evrope, postala tradicionalna. V teku so že priprave na konferenco IMTB 2012.

Konferenco sta v okviru dvostranskega znanstveno-raziskovalnega sodelovanja med Republiko Slovenijo in Republiko Hrvaško podprla Javna agencija za raziskovalno dejavnost Republike Slovenije in Ministrstvo za znanost, šolstvo in šport Republike Hrvaške. Glavna pokrovitelja dogodka sta bila Mettler Toledo in Donau Lab Ljubljana, ki sta med prireditvijo tudi predstavila proizvode s področja mikrostrukturiranih naprav, ostali sponzorji pa so bili BIA d.o.o., BIA Separations d.o.o., Helios, Tovarna barv, lakov in umetnih smol Količevo, d.o.o., Savatech d.o.o. in LPKF Laser & Elektronika d.o.o. Kot donatorji so konferenco finančno podprli še Atotech Slovenija d.d., Cinkarna Celje, d.d., Krka, tovarna zdravil, d.d., Melamin d.d. Kočevje in Pivovarna Union d.d.

Več na: http://imtb2010.fkkt.uni-lj.si.

VKLJUČENOST V OKOLJE

KEMIJSKA OLIMPIJADA 2010 V TOKYU

42. kemijska olimpijada je potekala od 19. 7. do 28. 7. 2010 v Tokyu. Gostili sta nas Univerza v Tokyu, kjer je potekalo tekmovanje iz teoretične kemije, in Univerza Waseda, kjer je potekal praktični del tekmovanja (http://www.icho2010.org/en/home.html). Predsedujoči olimpijade je bil Nobelov nagrajenec za kemijo 2001 profesor Ryoji Noyori.

Vsako državo lahko na olimpijadi zastopajo največ štirje tekmovalci, ki so bili najboljši na nacionalnem tekmovanju. Slovenijo je na tem tekmovanju zastopala naslednja ekipa: Žiga Perko in Božidar Aničić (oba II. gimnazija Maribor), Valter Bergant (Šolski center Rudolfa Maistra Kamnik) in Nejc Petek (gimnazija Litija). Mentorja slovenske ekipe sta bila dr. Andrej Godec in dr. Darko Dolenc s Fakultete za kemijo in kemijsko tehnologijo v Ljubljani, kjer potekajo tudi celoletne priprave mladih kemikov na to izredno zahtevno tekmovanje.

Na olimpijadi v Tokyu je sodelovalo 267 dijakov iz 68 držav.

Dijaki so imeli dva tekmovalna dneva. Najprej so morali v laboratoriju pokazati svoje praktične sposobnosti in izvesti tri praktične naloge: sintezo Hantzschevega estra in karakterizacijo s TLC; določevanje Fe(II) in Fe(III) v raztopini z vizualno kolorimetrično analizo; tretja naloga pa je bila analiza polisaharida, ki vsebuje sulfonatne ($–SO_3^-$) in karboksilatne

Slovenijo so na kemijski olimpijadi v Tokyu zastopali (od leve proti desni) Darko Dolenc (mentor), Božidar Aničić, Valter Bergant, Žiga Perko, Nejc Petek in Andrej Godec (mentor)

($-COO^-$) skupine, s koloidno titracijo v bazičnih in kislih pogojih. Za vse naloge so imeli skupaj 5 ur časa.

Drugi tekmovalni dan so morali reševati osem nalog, ki so zajemale vsa področja kemije; fizikalno kemijo in kvantno kemijo (plini, dovoljeni elektronski prehodi, hitrost zvoka, toplotna kapaciteta, fotoelektronska spektroskopija, termodinamika, litijeve ionske baterije), kristalografijo (kloridi in karbonati, Born Haberjev cikel), analizno kemijo (kemijska potreba po kisiku), in organsko kemijo (različne organske reakcije, izomerija, sinteza in struktura tetrodoksina – strupa Fugu rib napihovalk, esterifikacija, kondenzacijska polimerizacija, NMR spektroskopija). Naloge si lahko ogledate v spletni učilnici Kemljub, ki je namenjena tekmovanjem in našim dijakom; vanjo se morate prijaviti, vendar je prijava avtomatska (http://skupnost.sio.si/course/view.php?id=150).

Slovenska ekipa se je letos izvrstno odrezala: Žiga, Nejc in Valter so osvojili bronaste medalje, Božidar pa častno priznanje. Vsem čestitke!

Pri projektih za dijake sodeluje Zavod za šolstvo RS, in pri organizaciji udeležbe na olimpijadi Zveza za tehniško kulturo Slovenije. Kot donator pa nam pomaga podjetje BASF Slovenija d.o.o. Vsem se zahvaljujemo.

POLETNA ŠOLA KEMIJE 2010

V tednu od 28. 6. do 2. 7. 2010 je na Fakulteti za kemijo in kemijsko tehnologijo v Ljubljani potekala poletna šola kemije 2010. Gostili smo 17 dijakinj in dijakov iz cele Slovenije, ki so v tem tednu poglobili svoje znanje kemije in predvsem veliko delali v naših laboratorijih.

Poletno šolo kemije je organizirala naša fakulteta v sodelovanju z Zavodom RS za šolstvo in Zvezo za tehniško kulturo Slovenije.

Vodja poletne šole je bil dr. Andrej Godec, FKKT. Strokovno ekipo, ki je sodelovala pri izvedbi delavnic in predavanj, pa so sestavljali dr. Romana Cerc Korošec, dr. Helena Prosen, dr. Janez Cerkovnik (vsi FKKT) in mag. Andreja Bačnik, Zavod RS za šolstvo.

Udeleženke poletne šole 2010 pri delu v laboratoriju

Na začetku poletne šole so udeleženci poslušali predavanje o kemijski varnosti (mag. Andreja Bačnik), ki mu je sledila že prva praktična delavnica v laboratorijih katedre za analizno kemijo. Vodila jo je dr. Helena Prosen, pomagala pa ji je Mojca Žitko.

V tej delavnici so dijaki najprej s pomočjo redoks titracije s $KMnO_4$ določevali delež kisika (t.im. »aktivni kisik«) v komercialnih odstranjevalcih madežev. Zatem pa so z metodo plinske kromatografije v kombinaciji z masno spektrometrijo ugotavljali avtentičnost cvetlične dišave (eterično olje vrtnice) v nekaterih izdelkih.

Drugi dan poletne šole so dijaki dopoldne najprej obiskali Kemijski inštitut, kjer so si ogledali delo v izbranih laboratorijih. Zatem so na fakulteti poslušali predavanje Koliko kemije (dr. Andrej Godec), kjer so med drugim spoznavali omejitve pri pouku kemije v gimnazijah, in na praktičnih primerih možnost pridobivanja dodatnega kemijskega znanja z minimalno nadgradnjo obstoječih vsebin.

Popoldne je sledilo srečanje z našimi študenti, kjer so lahko iz prve roke dobili informacije o študiju kemije. Srečanje je pripravila Špela Primožič.

Tretji dan poletne šole je bila na vrsti delavnica iz anorganske kemije, ki je potekala v laboratoriju katedre za anorgansko kemijo. Delavnico je vodila dr. Romana Cerc Korošec, pomagal pa ji je Damjan Erčulj.

V tej delavnici so udeleženci najprej proučevali vplive na ravnotežne reakcije v raztopinah koordinacijskih ionov, in ugotavljali njihovo stabilnost. Zatem pa so sintetizirali še spojino $K_2[Cu(C_2O_4)_2]\cdot 2H_2O$, in jo delno okarakterizirali s titracijo s $KMnO_4$.

Četrtek so udeleženci preživeli v laboratoriju katedre za organsko kemijo. Delavnico je vodil dr. Janez Cerkovnik, pomagala pa mu je Zdenka Sakelšek.

Najprej je bila na vrsti izolacija maščob iz naravnih virov, ki je potekala s kontinuirno ekstrakcijo s Soxhletovim aparatom, in določevanje nenasičenih (dvojnih) vezi s titracijo s halogeni.

V naslednjem poskusu so udeleženci dokazovali prisotnost glukoze in škroba v sladkorjih.

Sledila je sinteza paracetamola, kontrola čistosti s kromatografijo, čiščenje s kristalizacijo in določevanje tališča čistega produkta.

Na koncu pa so dijaki sintetizirali še kafro, produkt pa so čistili s sublimacijo.

Poletno šolo smo zaključili v petek, 2. 7. 2010. Najprej smo slišali kratke predstavitve dejavnosti v laboratorijih in vtise, ki so jih pridobili dijaki v tem tednu; razvila se je tudi diskusija z mentorji.

Na tem mestu se še enkrat zahvaljujem strokovni ekipi in ostalim sodelavcem FKKT, ki so sodelovali pri izvedbi, ter obema partnerjema, Zavodu RS za šolstvo in Zvezi za tehniško kulturo Slovenije.

Leto 2011 je leto kemije, zato bo tudi poletna šola temu primerno obarvana.

NOČ ZNANSTVENIC IN ZNANSTVENIKOV 2010

V septembru 2010 je UL FKKT že petič priredila »Noč znanstvenic in znanstvenikov«, ki pa so jo nekateri že preimenovali – seveda neupravičeno – v »Noč čarovnic«. Na srečanje smo povabili otroške, mlade in malo starejše, pa tudi upokojene znanstvenice in znanstvenike. V okviru Direktorata za raziskave Evropske komisije je namreč po vsej Evropi potekal skupen dogodek »Reserchers' Night, 2010«. Šlo je za prikaz kemijskega eksperimentiranja in določenega kemijskega znanja in želeli smo, da bi kemijsko znanost na poljuden način približali vsem ljudem. Hkrati naj bi tudi naše mlajše generacije na tak, neposreden način navdušili za študij naravoslovnih in tehničnih vsebin, ki se jih večina mladine sedaj večinoma ogleduje virtualno na računalnikih.

Indukcijske sile med molekulami vode in ogljikovega dioksida

Dogodek naj bi v Evropski uniji potekal v okviru programa FP7 in je EU namenila za ta panevropski projekt kar 3.5 mio EUR. Na teh razpisih praviloma kemiki nismo uspešni, ker ponavadi zahtevamo premajhno vsoto denarja in ocenjevalci v Bruslju verjetno ne vedo, da ne moremo v našem okolju organizirati »mega« kemijskih dogodkov. Vendar smo kljub temu imeli svojo znanstveno noč že petič po vrsti v malo bolj skromnem obsegu. Pripravili smo vrsto tematsko obarvanih kemijskih poskusov (ognjenih, bruhajočih, pokajočih in svetlečih) in manjšo zakusko na koncu. Seveda z besedami težko opišemo kemijski poskus. Malce lažje se ga zapomniš, če vidiš ustrezno fotografijo ali kratek video. Še najlaže pa se ti vtisne v spomin, če poskus vidiš v živo – zaznaš blisk, slišiš eksplozijo. Odziv občinstva na prikazano eksperimentiranje je bil vzpodbuden.

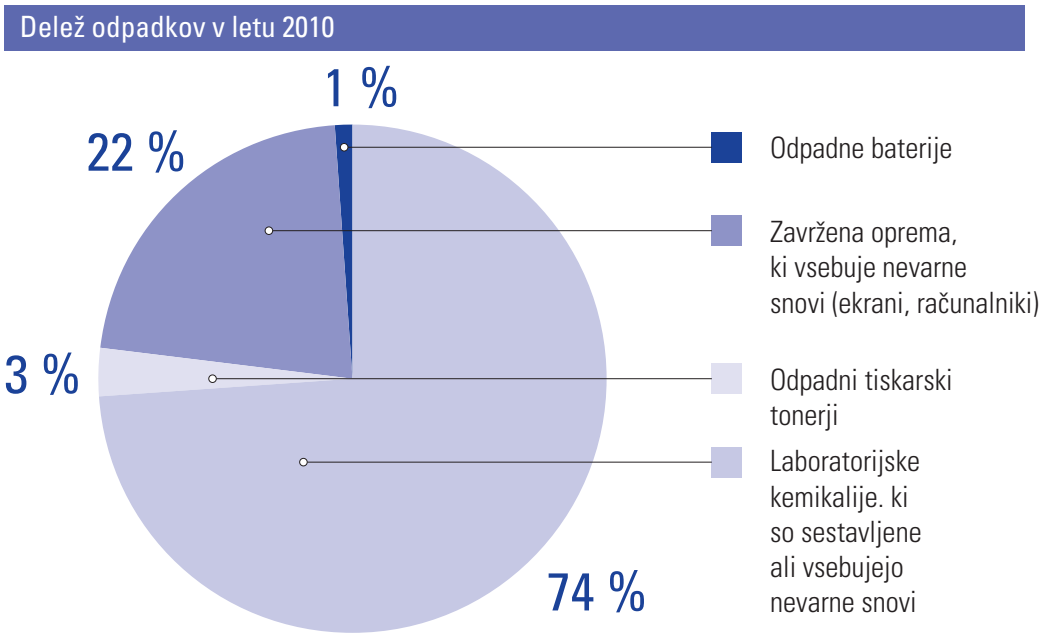
ZBIRANJE IN ODSTRANJEVANJE NEVARNIH ODPADKOV NA UL FKKT

Na fakulteti ločeno zbiramo naslednje skupine odpadkov:

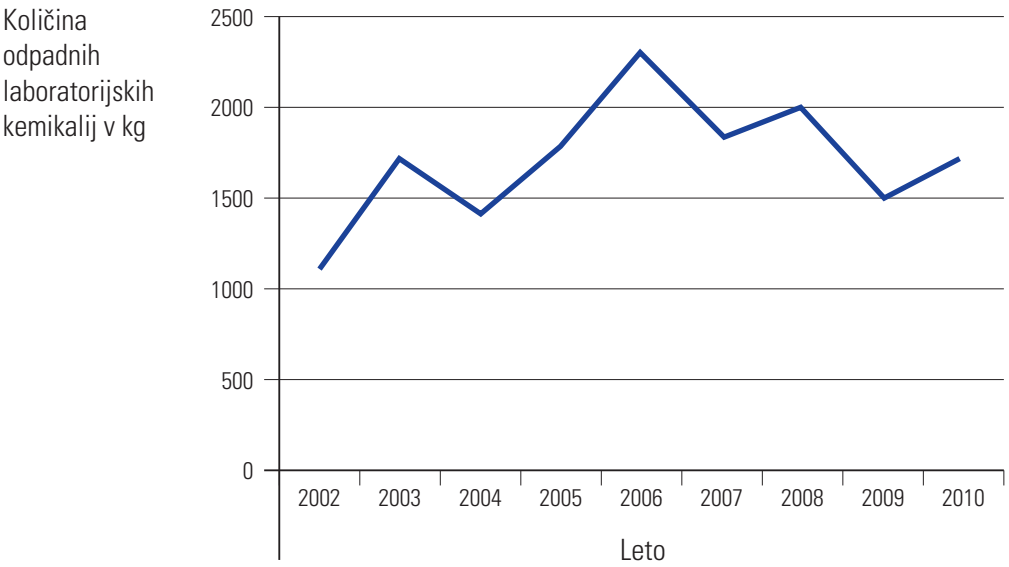
1. laboratorijske kemikalije, ki so sestavljene ali vsebujejo nevarne snovi
2. odpadni tiskarski tonerji
3. zavržena oprema, ki vsebuje nevarne snovi (računalniki, ekrani)
4. odpadne baterije.

Komunalni odpadki niso zajeti.

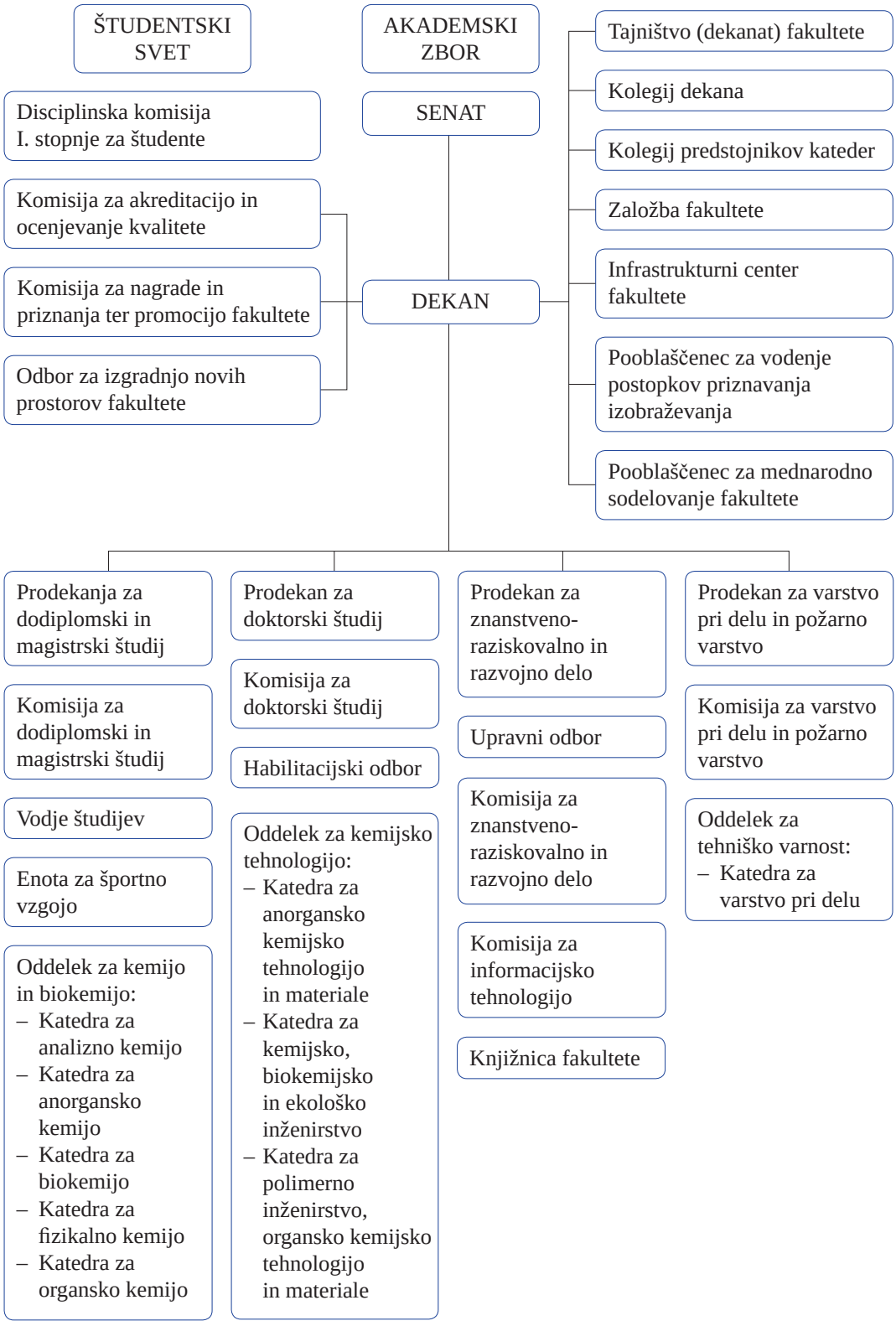
V spodnjem grafikonu je prikazan delež odpadkov po skupinah glede na količino v kg, zbranih v letu 2010.



Kot povzročitelji odpadkov moramo voditi evidenco o nastajanju odpadkov. V skladu z Uredbo o ravnanju z odpadki, poročilo o nastalih odpadkih vsako leto pošljemo Ministrstvu za okolje in prostor. Na spodnjem grafikonu je prikaz zbranih odpadnih laboratorijskih kemikalij v obdobju 2002–2010.



ORGANIZACIJSKA SHEMA



DIPLOME, MAGISTERIJI IN DOKTORATI V LETU 2010

DIPLOME

UNIVERZITETNI ŠTUDIJSKI PROGRAMI

KEMIJA

Miro Dobravc
Mentor: prof. dr. Darko Dolenc
Reakcije UV filtrov z oksidanti prisotnimi v naravnih vodah
Datum zagovora: 6. 7. 2010

Vanja Erjavec
Mentorica: doc. dr. Barbara Modec
Koordinacijske spojine s ksanturinsko kislino in njihova karakterizacija
Datum zagovora: 14. 10. 2010

Jan Fabris
Mentor: prof. dr. Andrej Petrič
Sinteza in karakterizacija novih azo analogov DDNP
Datum zagovora: 24. 2. 2010

Urban Feguš
Mentor: prof. dr. Jurij Svete
Sinteza 1-fenil-5-hidroksi-1*H*-pirazol-4-karboksamidov pod mikrovalovi
Datum zagovora: 8. 7. 2010

Neža Furlan
Mentor: prof. dr. Peter Bukovec
Kemijska speciacija kompleksov platine s protitumorskim delovanjem v krvnem serumu
Datum zagovora: 8. 6. 2010

Petra Horvat
Mentorica: doc. dr. Romana Cerc Korošec
Optimizacija fotokatalitske učinkovitosti tankih plasti in prahov titanovega dioksida, pripravljenih po sol-gel postopku
Datum zagovora: 19. 10. 2010

Irena Hrovat
Mentor: prof. dr. Peter Bukovec
Sinteza in karakterizacija kovinskih kompleksov s ksanturinsko kislino in drugimi ligandi
Datum zagovora: 26. 10. 2010

Tanja Koleša
Mentor: akademik prof. dr. Branko Stanovnik
[2+2] Cikloadicije (dimetilamino)enaminonov na dimetil acetilendikarboksilat
Datum zagovora: 15. 6. 2010

Andrej Kovič
Mentor: prof. dr. Iztok Turel
Sinteza in karakterizacija novih rutenijevih organokovinskih spojin
Datum zagovora: 14. 9. 2010

Vesna Kren
Mentorica: doc. dr. Helena Prosen
Razvoj metode za določevanje fenolnih spojin v čajih
Datum zagovora: 16. 9. 2010

Marko Krivec
Mentor: prof. dr. Marijan Kočevar
Uporaba heterogenih katalizatorjev pri pripravi izoindolov iz izbranih 2*H*-piran-2-onov
Datum zagovora: 13. 9. 2010

Uroš Kvenderc
Mentorica: doc. dr. Nina Lah
Koordinacijske spojine bakra z enostavnimi piridinskimi alkoholi
Datum zagovora: 8. 6. 2010

Ilza Marković
Mentor: prof. dr. Boris Pihlar
Validacija kulometrične metode za določevanje vode v citronski kislini
Datum zagovora: 27. 9. 2010

Andrej Mernik
Mentor: prof. dr. Jurij Lah
Termodinamika vezanja antitoksina CcdA na toksin CcdB iz bakterije *Vibrio fischeri*
Datum zagovora: 15. 6. 2010

Jernej Pavlič
Mentor: prof. dr. Anton Meden
Priprava in karakterizacija debelih plasti na osnovi (K,Na)NbO_3
Datum zagovora: 24. 6. 2010

Peter Perdih
Mentor: prof. dr. Jurij Svete
Paralelna sinteza novih pirazolovih analogov histamina
Datum zagovora: 31. 8. 2010

Rok Prebil
Mentor: prof. dr. Jurij Svete
Reakcije benzofenona in nitrofenilpirazola z elektrofili
Datum zagovora: 31. 8. 2010

Marta Pregl
Mentor: prof. ddr. Boris Turk
Priprava fuzijskih proteinov katepsinov D in E s proteinom GST
Datum zagovora: 13. 4. 2010

Sandra Prešeren
Mentorica: prof. dr. Metka Renko
Razvoj metode za določevanje aktivnosi aminopeptidaze N v urinu
Datum zagovora: 8. 6. 2010

Kristian Radan
Mentor: prof. dr. Alojz Demšar
Spojine nekaterih dvovalentnih kovin z dvojnimi perfluoro anioni
Datum zagovora: 13. 9. 2010

Peter Rodič
Mentorica: prof. dr. Barbara Hribar Lee
Koncentracijska odvisnost transportnih števil v vodnih raztopinah ionen bromidov
Datum zagovora: 3. 9. 2010

Rok Rudež
Mentor: doc. dr. Drago Kočar
Somentorica: doc. dr. Ida Poljanšek
Sinteza in karakterizacija dendrimera 2. generacije iz glikolne in 2,2-dimetilpropijonske kisline
Datum zagovora: 27. 10. 2010

Ivo Ruperčič
Mentor: prof. dr. Peter Bukovec
Sinteza in karakterizacija kompleksov kovin prehoda in ksanturinske kisline
Datum zagovora: 6. 10. 2010

Anja Sirk
Mentorica: doc. dr. Romana Cerc Korošec
Somentorica: dr. Polona Umek, znanstvena sodelavka
Vpliv vsebnosti kalija na termično stabilnost α-MnO_2
Datum zagovora: 4. 2. 2010

Maja Vidmar
Mentorica: doc. dr. Amalija Golobič
Kvantitativna fazna analiza zmesi trdnin z različnimi metodami praškovne difrakcije
Datum zagovora: 9. 9. 2010

Katarina Vrhovec
Mentorica: prof. dr. Lucija Zupančič-Kralj
Vpeljava pasivnega vzorčenja za določevanje zdravilnih učinkovin v vodah
Datum zagovora: 19. 5. 2010

Nina Žibert
Mentor: prof. dr. Peter Bukovec
Zamreževanje fenol-formaldehidnih, novolačnih smol s heksametilentetraminom
Datum zagovora: 8. 9. 2010

KEMIJSKO IZOBRAŽEVANJE

Tadeja Birsa Čelić
Mentorica: doc. dr. Amalija Golobič
Somentor: prof. dr. Venčeslav Kaučič
Sinteza in strukturna karakterizacija poroznih železovih karboksilatov
Datum zagovora: 19. 5. 2010

Rok Rudež
Mentor: doc. dr. Drago Kočar
Somentorica: doc. dr. Ida Poljanšek
Sinteza in karakterizacija dendrimera 2. generacije iz glikolne in 2,2-dimetilpropijonske kisline
Datum zagovora: 27. 10. 2010

Anja Sirk
Mentorica: doc. dr. Romana Cerc Korošec
Somentorica: dr. Polona Umek, znanstvena sodelavka
Vpliv vsebnosti kalija na termično stabilnost α-MnO_2
Datum zagovora: 4. 2. 2010

Katarina Vrhovec
Mentorica: prof. dr. Lucija Zupančič-Kralj
Vpeljava pasivnega vzorčenja za določevanje zdravilnih učinkovin v vodah
Datum zagovora: 19. 5. 2010

BIOKEMIJA

Tina Berk
Mentor: prof. dr. Peter Bukovec
Anaerobna razgradnja glukoze v prisotnosti cianidov
Datum zagovora: 17. 11. 2010

Sabina Božič
Mentor: prof. dr. Roman Jerala
Priprava rekombinantnega polipeptida iz obvitih vijačnic za tvorbo nanostruktur
Datum zagovora: 8. 9. 2010

Simon Buček
Mentorica: prof. dr. Tatjana Avšič-Županc
Razvoj metode verižne reakcije s polimerazo v realnem času za dokazovanje virusa Zahodnega Nila v vzorcih ptic
Datum zagovora: 9. 7. 2010

Adriana Damjanović
Mentor: doc. dr. Marko Dolinar
Genetsko inženirstvo genoma mišjega citomegalovirusa za ustvarjanje virusnih sevov Δm160, Δm161 in Δm162 na osnovi rekombinacije
Datum zagovora: 18. 10. 2010

Tanja Dolinšek
Mentor: prof. dr. Janko Kos
Somentor: prof. dr. Gregor Serša
Vpliv utišanja endoglina na preživetje humanih endotelnih celic Hmec-1 *in vitro*
Datum zagovora: 2. 7. 2010

Sara Drmota
Mentorica: prof. dr. Tamara Lah Turnšek
Invazivnost normalnih in tumorskih matičnih celic možganov
Datum zagovora: 22. 6. 2010

Taja Glivar
Mentor: prof. dr. Peter Bukovec
Določevanje sestave bioplina pri anaerobni razgradnji glukoze v prisotnosti cianidnih ionov
Datum zagovora: 8. 6. 2010

Katja Goričar
Mentorica: prof. dr. Ana Plemenitaš
Somentorica: prof. dr. Vita Dolžan
Genetski polimorfizmi encimov za popravljanje napak na DNA s homologno rekombinacijo v zdravi slovenski populaciji in njihov vpliv na stopnjo poškodb DNA
Datum zagovora: 22. 6. 2010

Matej Jereb
Mentor: prof. dr. Igor Križaj
Somentor: doc. dr. Uroš Petrovič
Od cinka odvisne genetske interakcije homologa adiponektinskega receptorja kvasovke z z G-proteini povezanimi geni
Datum zagovora: 9. 7. 2010

Saša Jereb
Mentor: prof. dr. Igor Križaj
Razvoj od mutacij neodvisnega zaznavanja virusa HIV
Datum zagovora: 27. 8. 2010

Maria Juretić
Mentorica: prof. dr. Metka Renko
Zaščitni učinek polifenolov iz kakava na z CCl_4 povzročeno poškodbo jeter
Datum zagovora: 27. 8. 2010

Matejka Juvančič
Mentor: prof. dr. Igor Križaj
Priprava in karakterizacija dimerov cisteinskih analogov filgrastima
Datum zagovora: 1. 10. 2010

Marija Kokalj
Mentorica: prof. dr. Vladka Čurin Šerbec
Uporaba verižne reakcije s polimerazo za kvantifikacijo bakteriofagov
Datum zagovora: 27. 7. 2010

Matic Krivec
Mentorica: doc. dr. Polona Žnidaršič Plazl
Proizvodnja L–jabolčne kisline v mikrokanalih z imobilizirano kvasovko *Saccharomyces cerevisiae*
Datum zagovora: 15. 6. 2010

Jan Lonzarić
Mentor: prof. dr. Roman Jerala
Priprava genskega cepiva za aktivacijo prirojene in pridobljene imunosti
Datum zagovora: 7. 9. 2010

Anja Lukan
Mentor: doc. dr. Marko Dolinar
Analiza občutljivosti testa na osnovi mRNA za določanje menstrualne krvi in vaginalnih izločkov v bioloških sledeh
Datum zagovora: 1. 9. 2010

Anže Martinčič
Mentorica: doc. dr. Polona Žnidaršič Plazl
Preučitev možnosti pridobivanja bioetanola iz izbranih industrijskih odpadkov
Datum zagovora: 14. 4. 2010

Nataša Medved
Mentor: prof. dr. Roman Jerala
Vpliv znotrajcelične vrednosti pH in koncentracije kalcija na delovanje protiglivnih substanc pri glivi *Aspergillus niger*
Datum zagovora: 14. 4. 2010

Judita Merzdovnik
Mentor: prof. dr. Radovan Komel
Priprava rekombinantne parabenzoatne hidroksilaze za kristalizacijske študije
Datum zagovora: 1. 10. 2010

Ana Miklavžin
Mentor: prof. ddr. Boris Turk
Priprava deglikoziliranih mutant lizosomske dipeptidaze v sesalskih celicah HEK 293
Datum zagovora: 22. 1. 2010

Robert Novak
Mentorica: doc. dr. Helena Prosen
Primerjava ekstrakcijskih tehnik za analizo eteričnih olj v različnih matricah
Datum zagovora: 25. 2. 2010

Urban Novak
Mentor: prof. dr. Janez Plavec
Strukturne analize hidratiranega Konkanavalina A z uporabo infrardeče spektroskopije
Datum zagovora: 25. 11. 2010

Jernej Oberčkal
Mentor: prof. dr. Igor Križaj
Identifikacija vezavnih proteinov za amoditoksin C v sesalskih nevronskih celicah
Datum zagovora: 8. 9. 2010

Matevž Ogrizek
Mentorica: prof. dr. Brigita Lenarčič
Kloniranje in izražanje zunajceličnih domen proteinov Trop1 in Trop2
Datum zagovora: 8. 4. 2010

Nada Simončič
Mentorica: doc. dr. Andreja Žgajnar Gotvajn
Določanje strupenosti snovi in odpadnih vod z višjimi rastlinami
Datum zagovora: 13. 12. 2010

Matej Somrak
Mentor: prof. dr. Igor Križaj
Somentor: doc. dr. Uroš Petrovič
Identifikacija interaktorjev proteina Pex11 kvasovke *Saccharomyces cerevisiae* z metodo tandemskega afinitetnega čiščenja
Datum zagovora: 9. 7. 2010

Andreja Šober
Mentorica: prof. dr. Lucija Zupančič-Kralj
Določanje vsebnosti furana v termično obdelanih živilih
Datum zagovora: 25. 2. 2010

Vladimir Vajda
Mentorica: prof. dr. Metka Renko
Razvoj metode za določevanje citotoksičnosti polistirenskih nanodelcev
Datum zagovora: 29. 1. 2010

Robert Vidmar
Mentorica: prof. dr. Lucija Zupančič-Kralj
Razvoj peptidne karte za določanje istovetnosti terapevtskega proteina
Datum zagovora: 17. 9. 2010

Tilen Vidmar
Mentorica: prof. dr. Brigita Lenarčič
Priprava in karakterizacija tiroglobulinskih domen tipa 1 testikanov-2 in -3
Datum zagovora: 7. 9. 2010

Tina Zupančič
Mentor: prof. dr. Radovan Komel
Razvoj in vrednotenje *in vitro* modela črevesnega epitelija za testiranje prehajanja proteinov
Datum zagovora: 1. 10. 2010

Neja Zupanec
Mentor: prof. dr. Radovan Komel
Funkcijska analiza petih različic gena *hMLH1* v kvasovki *Saccharomyces cerevisiae*
Datum zagovora: 7. 4. 2010

KEMIJSKO INŽENIRSTVO

Vida Alič
Mentor: prof. dr. Miran Gaberšček
Dvostopenjska sinteza in elektrokemijska karakterizacija $LiVPO_4F$, kot katodnega materiala za litijeve baterije
Datum zagovora: 10. 9. 2010

Irena Bergant
Mentor: prof. dr. Matjaž Kranjc
Dinamična mehanska analiza in karakterizacija napak pri utrujanju plošč tiskanih vezij
Datum zagovora: 25. 2. 2010

Andrej Bobnar
Mentorica: doc. dr. Andreja Žgajnar Gotvajn
Primerjava različnih metod čiščenja deponijskih izcednih vod
Datum zagovora: 22. 12. 2010

Suzana Bošković
Mentor: prof. dr. Marin Berovič
Uporaba magnetnih nanodelcev za separacijo kvasovk *Saccharomyces cerevisiae* v alkoholni fermentaciji
Datum zagovora: 23. 6. 2010

Ana Cankar
Mentorica: doc. dr. Andreja Zupančič Valant
Priprava gumirane asfaltne zmesi po mokrem in suhem postopku
Datum zagovora: 29. 6. 2010

Helena Fajfar
Mentor: prof. dr. Janvit Golob
Optimizacija nizkotemperaturnega izparevanja za določitev radioaktivnosti
Datum zagovora: 7. 10. 2010

Ana Gantar
Mentor: prof. dr. Marin Berovič
Modeliranje kultivacije biomase glive *Grifola frondosa* na trdnem gojišču
Datum zagovora: 15. 7. 2010

Danijel Gazvoda
Mentor: prof. dr. Marin Berovič
Uporaba fizikalnih in kemijskih dejavnikov stresa za izolacijo odpornih linij *Streptomices sp*.
Datum zagovora: 29. 6. 2010

Jan Geder
Mentor: prof. dr. Matjaž Krajnc
Adsorpcijsko razžveplanje srednjih destilatov za uporabo v gorivnih celicah
Datum zagovora: 7. 10. 2010

Miha Kavšek
Mentor: doc. dr. Blaž Likozar
Mikroenkapsulacija insekticida s polimerno membrano
Datum zagovora: 17. 9. 2010

Maja Kerovec
Mentor: prof. dr. Marin Berovič
Vpliv procesnih parametrov na biosintezo polimera PHA
Datum zagovora: 15. 9. 2010

Maša Kodela
Mentor: prof. dr. Marin Berovič
Biosinteza ergosterola in polisaharidov v glivi *Grifola frondosa*
Datum zagovora: 1. 10. 2010

Urška Košnik
Mentorica: doc. dr. Urška Šebenik
Inkapsulacija butil stearata z melaminsko-formaldehidno smolo
Datum zagovora: 15. 7. 2010

Branko Lah
Mentor: prof. dr. Marin Berovič
Uporaba glive *Trichoderma reesei* za razgradnjo lignocelulozne biomase
Datum zagovora: 7. 10. 2010

Domen Lapornik
Mentor: doc. dr. Blaž Likozar
Ravnotežje in prenos snovi pri sušenju agarnih gelov za pripravo rodenticida
Datum zagovora: 29. 9. 2010

Alenka Likar
Mentorica: doc. dr. Klementina Zupan
Materiali za enoprostorske gorivne celice s trdnim elektrolitom
Datum zagovora: 3. 6. 2010

Martin Lubej
Mentor: prof. dr. Igor Plazl
Sinteza ogljikovih nanocevk
Datum zagovora: 14. 9. 2010

Miodrag Mitrović
Mentor: prof. dr. Matjaž Kranjc
Protikorzijske lastnosti organsko-anorganskih hibridov z vključenimi organskimi inhibitorji
Datum zagovora: 25. 2. 2010

Boštjan Nograšek
Mentor: doc. dr. Blaž Likozar
Načrtovanje integriranega procesa oplaščanja zrn umetnih gnojil in sušenja s fluidiziranim slojem
Datum zagovora: 26. 8. 2010

Aleš Novak
Mentorica: doc. dr. Klementina Zupan
Kompoziti na osnovi sistema Fe-Al
Datum zagovora: 3. 6. 2010

Uroš Novak
Mentorica: doc. dr. Polona Žnidaršič Plazl
Encimsko katalizirana transesterifikacija v mikroreaktorju s strnjenim slojem
Datum zagovora: 15. 7. 2010

Alenka Okršlar
Mentor: doc. dr. Marjan Marinšek
Priprava paladijevega katalizatorja na ogljikovem nosilcu za nizkotemperaturno gorivno celico z direktno uporabo mravljinčne kisline
Datum zagovora: 22. 4. 2010

Matjaž Pevec
Mentorica: doc. dr. Andreja Žgajnar Gotvajn
Adsorpcija bisfenola A med Fentonovo oksidacijo
Datum zagovora: 2. 4. 2010

Robert Pivar
Mentor: doc. dr. Blaž Likozar
Analiza tehnoloških procesov od parnega reforminga do proizvodnje formaldehida
Datum zagovora: 4. 11. 2010

Petra Sečnik
Mentorica: prof. dr. Jana Zagorc Končan
Čiščenje deponijskih izcednih vod z adsorpcijo
Datum zagovora: 22. 12. 2010

Stanka Smrdelj Musić
Mentorica: doc. dr. Urška Šebenik
Vpliv procesnih pogojev na strukturo in zamreževanje sečninsko-formaldehidnih smol
Datum zagovora: 15. 10. 2010

Andreja Šestan
Mentorica: doc. dr. Klementina Zupan
Mikrostrukturne karakteristike materialov na osnovi Ni-GDC in GDC pripravljenih po citratno nitratnem zgorevalnem postopku
Datum zagovora: 24. 9. 2010

Matej Špec
Mentor: prof. dr. Igor Plazl
Ločevanje snovi od ionskih kapljevin z uparevanjem v miniaturizirani napravi
Datum zagovora: 24. 9. 2010

Živa Švab
Mentorica: doc. dr. Andreja Zupančič Valant
Vpliv temperature in dodatka volumskih ekspanderjev na reološke lastnosti krvi
Datum zagovora: 11. 2. 2010

Anita Tavčar
Mentorica: doc.dr. Urška Šebenik
Vpliv vrste emulgatorja na šaržno polimerizacijo oktametilciklotetrasiloksana v emulziji
Datum zagovora: 21. 10. 2010

Darja Teslić
Mentorica: doc. dr. Urška Šebenik
Sinteza nanokompozitnih UV zamrežljivih akrilatnih lepil
Datum zagovora: 15. 7. 2010

Ilija Trajkovski
Mentor: prof. dr. Marin Berovič
Produkcija biomase in polisaharidov glive *Grifola frondosa* v mešalnem reaktorju in v koloni z mehurčki
Datum zagovora: 1. 10. 2010

Živa Trtnik
Mentorica: doc. dr. Klementina Zupan
Zgoščevanje natrijevega niobata pripravljenega s mehanokemijsko sintezo
Datum zagovora: 21. 10. 2010

Teja Urbas
Mentor: prof. dr. Matjaž Krajnc
Ionske tekočine kot prevodniki v elektro in elektrooptičnih sistemih
Datum zagovora: 16. 6. 2010

Žiga Velišček
Mentor: prof. dr. Radovan Stanislav Pejovnik
Priprava in karakterizacija zlitin v sistemu litij-bor
Datum zagovora: 26. 2. 2010

VISOKOŠOLSKA ŠTUDIJSKA PROGRAMA

KEMIJSKA TEHNOLOGIJA

Suzana Ambrožič Radkovič
Mentorica: doc. dr. Helena Prosen
Somentor: doc. dr. Blaž Cigić
Določanje vezave barvil iz odpadnih vod na sorbente s spektrofotometrično metodo
Datum zagovora: 17. 6. 2010

Elena Arsova
Mentor: prof. dr. Marjan Veber
Optimizacija postopka za elementno analizo vzorcev odpadne plastike z ICP-AES in ICP-MS
Datum zagovora: 1. 2. 2010

Gregor Avbelj
Mentor: doc. dr. Marjan Marinšek
Nano disperzije paladija na ogljikovih nanocevkah za nizkotemperaturne DFAFC gorivne celice
Datum zagovora: 6. 1. 2010

Tanja Bačnik
Mentorica: prof. dr. Nataša Gros
Določanje nizkih koncentracij etanola v živilskih vzorcih
Datum zagovora: 26. 10. 2010

Monika Brezovar
Mentor: prof. dr. Radovan Stanislav Pejovnik
Študij vpliva parametrov kristalizacije na velikost delcev produkta
Datum zagovora: 17. 6. 2010

Margareta Cof
Mentor: prof. dr. Marjan Veber
Somentorica: prof. dr. Marija Bogataj
Sproščanje natrijevega dikofenakata iz Voltaren tablet
Datum zagovora: 1. 7. 2010

Katja Čeh
Mentorica: doc. dr. Ana Lakota
Spremljanje poteka biološke denitrifikacije z in- situ merilniki
Datum zagovora: 30. 11. 2010

Mateja Černevšek
Mentorica: doc. dr. Urška Šebenik
Vpliv polivinilalkoholov na barierne premaze papirja
Datum zagovora: 12. 11. 2010

Sabina Drnovšek
Mentorica: prof. dr. Nataša Gros
Določanje vsebnosti vodotopnih kloridov v historičnih materialih
Datum zagovora: 26. 10. 2010

Ema Fabjan
Mentorica: doc. dr. Urška Šebenik
Vpliv izocianatnega indeksa na lastnosti poliuretanskih pen iz utekočinjenega lesa
Datum zagovora: 6. 7. 2010

Barbara Ferenčak
Mentor: prof. dr. Marjan Veber
Validacija spektrofotometrične metode za določevanje Cr(VI) v vodi in aerosolnih delcih
Datum zagovora: 26. 1. 2010

Tatjana Filipič
Mentor: doc. dr. Bogdan Štefane
Somentor: doc. dr. Janez Kovač
Priprava in karakterizacija tankih organskih monoplasti na SiO_2
Datum zagovora: 7. 12. 2010

Primož Flajs
Mentor: prof. dr. Matjaž Krajnc
Utrjevanje epoksi premazov na vodni osnovi
Datum zagovora: 14. 12. 2010

Luka Gornik
Mentor: doc. dr. Marjan Marinšek
Pd-disperzije na ogljikovih nanocevkah za anode nizkotemperaturnih gorivnih celic z direktno uporabo metanojske kisline ali metanola
Datum zagovora: 7. 4. 2010

Irena Hace
Mentor: doc. dr. Franc Perdih
Sinteza in karakterizacija spojin organtitanovih fluoridov s sulfatnim ligandom
Datum zagovora: 20. 10. 2010

Damjana Ilar
Mentor: prof. dr. Marjan Veber
Primerjava točnosti priprav za merjenje prostornine
Datum zagovora: 21. 12. 2010

Žiga Klemenšek
Mentorica: doc. dr. Helena Prosen
Validacija HPLC metode za določevanje nečistot Bacitracina v farmacevtskem izdelku
Datum zagovora: 27. 9. 2010

Marinka Korevec
Mentorica: prof. dr. Jana Zagorc Končan
Respiracijska aktivnost mehansko-biološko obdelanih odpadkov
Datum zagovora: 12. 11. 2010

Blaž Kuhar
Mentorica: viš. pred. mag. Barbara Novosel
Odstranjevanje nanosov ogljika z anodnega SOFC materiala
Datum zagovora: 29. 10. 2010

Karmen Lampreht
Mentorica: prof. dr. Nataša Gros
Spektrometrično spremljanje mikrodifuzije hlapnih komponent v Conway-evi celici pri različnih temperaturah
Datum zagovora: 2. 9. 2010

Tanja Lampreht Štravs
Mentorica: prof. dr. Nataša Gros
Spektrometrično merjenje v miniaturiziranih sistemih
Datum zagovora: 19. 1. 2010

Nevenka Lilik
Mentor: prof. dr. Marjan Veber
Somentor: prof. dr. Albin Kristl
Nespecifična vezava nekaterih učinkovin na laboratorijske materiale pri določanju permeabilnosti
Datum zagovora: 30. 11. 2010

Črtomir Martinjak
Mentor: doc. dr. Marjan Marinšek
Priprava nano paladijevih disperzij na ogljikovih nosilcih
Datum zagovora: 2. 12. 2010

Mateja Matko
Mentorica: prof. dr. Lucija Zupančič-Kralj
Določanje ostankov učinkovine iz skupine alkaloidov na proizvodni opremi
Datum zagovora: 27. 9. 2010

Zdenka Mauser
Mentorica: prof. dr. Nataša Gros
Določanje vitamina D v krmi in krmnih dodatkih
Datum zagovora: 17. 5. 2010

Robert Mesojednik
Mentor: prof. dr. Aleksander Pavko
Izolacija farmacevtskih učinkovin iz organskih topil z nanofiltracijsko membrano Duramem 200
Datum zagovora: 17. 9. 2010

Mohor Mihelčič
Mentor: prof. dr. Matjaž Krajnc
Somentor: prof. dr. Boris Orel
Poliedrični oligomerni silseskvioksani za modifikacijo pigmentov v spektralno selektivnih premazih
Datum zagovora: 22. 9. 2010

Uroš Mohar
Mentor: prof. dr. Matjaž Krajnc
Optimizacija sinteze, izolacije in stereoselektivnih kristalizacijskih pogojev za kiralni heterociklični intermediat pri sintezi novega antilipidemika
Datum zagovora: 17. 6. 2010

Andreja Sobočan
Mentorica: doc. dr. Urška Šebenik
Vpliv sestave akrilatnega prepolimera na lastnosti UV zamrežljivih PSA lepil
Datum zagovora: 18. 3. 2010

Alenka Steklasa
Mentorica: doc. dr. Saša Petriček
Kompleksi kovinskih halogenidov z etri
Datum zagovora: 21. 4. 2010

Matjaž Strmec
Mentorica: doc. dr. Helena Prosen
Določanje dodanih umetnih arom v vinih
Datum zagovora: 26. 2. 2010

Mateja Suhodolčan
Mentorica: doc. dr. Klementina Zupan
Kvantitativna analiza mikrostrukture anodnih materialov za visokotemperaturne gorivne celice na osnovi kompozita Ni – YSZ
Datum zagovora: 26. 8. 2010

Matej Škvarč
Mentor: prof. dr. Jadran Maček
Priprava elektrod, sestavljanje in testiranje alkalne gorivne celice
Datum zagovora: 29. 9. 2010

Petra Šutar
Mentor: doc. dr. Marjan Marinšek
Priprava nanodelcev cinkovega sulfida
Datum zagovora: 8. 11. 2010

Tonček Trbanc
Mentorica: doc. dr. Ana Lakota
Študij obratovalnih parametrov procesa adsorpcije vankomicina v ekspandiranem sloju
Datum zagovora: 5. 2. 2010

Katja Vovko
Mentorica: prof. dr. Nataša Gros
Določanje sladkorjev v vinu s tekočinsko kromatografijo visoke ločljivosti
Datum zagovora: 15. 12. 2010

Petra Vrbinc
Mentorica: prof. dr. Nataša Gros
Določanje sestave citratnega pufra v epruvetah za koagulacijske preiskave
Datum zagovora: 2. 9. 2010

Tomaž Vrtačič
Mentorica: doc. dr. Klementina Zupan
Oksidni anodni materiali na osnovi lantanovega kromit manganita za SOFC
Datum zagovora: 27. 10. 2010

Petra Žnidaršič
Mentorica: prof. dr. Nataša Gros
Določanje citrata v pufernih raztopinah z volumetrično titracijo
Datum zagovora: 7. 12. 2010

VARSTVO PRI DELU IN POŽARNO VARSTVO

Drago Ahlin
Mentor: prof. dr. Marjan Bilban
Somentor: viš. pred. dr. Jože Šrekl
Sindrom karpalnega kanala pri delu z računalnikom
Datum zagovora: 25. 11. 2010

Marko Ajdič
Mentor: pred. mag. Aleš Jug
Evakuacija iz bolnišnice
Datum zagovora: 25. 11. 2010

Marko Ban
Mentor: pred. mag. Aleš Jug
Krmiljenje požarnih vrat na evakuacijskih poteh
Datum zagovora: 14. 10. 2010

Anže Boh
Mentor: pred. mag. Aleš Jug
Izbor gasilnika glede na vrsto gorljivih snovi
Datum zagovora: 15. 7. 2010

Peter Cafuta
Mentor: doc. dr. Mitja Kožuh
Pasivna hiša
Datum zagovora: 15. 12. 2010

Andrej Čebela
Mentorica: viš. pred. mag. Barbara Novosel
Zagotavljanje varnosti pri klor-alkalnem procesu
Datum zagovora: 31. 8. 2010

Sebastijan Dodič
Mentorica: viš. pred. mag. Barbara Novosel
Somentor: pred. mag. Aleš Jug
Ukrepi za izboljšanje varnosti in zdravja pri delu s kemikalijami v lakirnici in analiza razvoja požara
Datum zagovora: 17. 6. 2010

Andrej Feguš
Mentor: doc. dr. Boris Jerman
Varno delo s stroji težke gradbene mehanizacije
Datum zagovora: 22. 4. 2010

Nataša Femec
Mentor: prof. dr. Andrej Polajnar
Ergonomska analiza pisarniškega delovnega mesta
Datum zagovora: 26. 5. 2010

Primož Fridrih
Mentor: doc. dr. Mitja Kožuh
Čiščenje voda z rastlinskimi čistilni napravami
Datum zagovora: 15. 12. 2010

Sebastijan Gauš
Mentorica: viš. pred. mag. Barbara Novosel
Varno skladiščenje nevarnih kemikalij
Datum zagovora: 22. 10. 2010

Katja Gorišek
Mentor: doc. dr. Mitja Kožuh
Večje tehnološke nesreče in varnostna kultura
Datum zagovora: 15. 12. 2010

Gregor Gorjup
Mentor: doc. dr. Mitja Kožuh
Gorivna celica
Datum zagovora: 15. 7. 2010

Gregor Gričnik
Mentor: doc. dr. Mitja Kožuh
Osveščanje ljudi o ravnanju z odpadno embalažo
Datum zagovora: 31. 8. 2010

Peter Hrovat
Mentor: doc. dr. Mitja Kožuh
Uvedba sistema ravnanja z okoljem po standardu SIST EN ISO 14001 v gradbeno industrijo
Datum zagovora: 7. 7. 2010

Melita Jamnik
Mentor: doc. dr. Mitja Kožuh
Varno delo in gibanje ob vodi
Datum zagovora: 6. 6. 2004

Vinko Jenko
Mentor: viš. pred. dr. Jožef Horvat
Osebna varovalna oprema gasilca in varnostni načrt z oceno tveganja
Datum zagovora: 15. 12. 2010

Stanislav Knap
Mentor: doc. dr. Mitja Kožuh
Program varstva okolja v občini Brezovica
Datum zagovora: 31. 3. 2010

Simona Kokelj
Mentorica: viš. pred. mag. Barbara Novosel
Varno in zdravo delo v konservatorskih-restavratorskih delavnicah
Datum zagovora: 22. 12. 2010

Dane Kos
Mentor: doc. dr. Grega Bizjak
Zaščita in varstvo pri delu na elektroenergetskih postrojih
Datum zagovora: 15. 7. 2010

Petra Lavrin
Mentor: doc. dr. Mitja Kožuh
Celovito ravnanje z odpadki in nevarnimi gospodinjskimi odpadki
Datum zagovora: 7. 7. 2010

Marko Lemut
Mentor: doc. dr. Mitja Kožuh
Pokrivanje energetskih potreb Republike Slovenije
Datum zagovora: 15. 7. 2010

Matic Leskovec
Mentor: viš. pred. dr. Jožef Horvat
Osebna varovalna oprema na delovnem mestu prodajalec – hladni program
Datum zagovora: 22. 10. 2010

Janez Levec
Mentor: doc. dr. Mitja Kožuh
Celovito ravnanje z odpadki
Datum zagovora: 15. 7. 2010

David Levovnik
Mentor: doc. dr. Mitja Kožuh
Varnost vodikovih tehnologij
Datum zagovora: 15. 7. 2010

Matej Ličan
Mentor: pred. mag. Aleš Jug
Požari osebnih vozil
Datum zagovora: 23. 9. 2010

Katarina Lipovnik
Mentorica: prof. dr. Marija Bešter Rogač
Pomen meritev prašnih emisij pri ocenjevanju tveganj in verifikacija aktualnih ukrepov varnosti in zdravja pri delu
Datum zagovora: 22. 12. 2010

Mojca Lunar
Mentor: pred. mag. Aleš Jug
Požarna problematika v obratu
Datum zagovora: 26. 5. 2010

Rok Mahne
Mentor: doc. dr. Mitja Kožuh
Ločeno zbiranje in transport odpadkov
Datum zagovora: 31. 8. 2010

Blaž Mavrič
Mentor: viš. pred. dr. Jožef Horvat
Somentor: viš. pred. dr. Jože Šrekl
Varnost na smučiščih in priporočena osebna varovalna oprema
Datum zagovora: 31. 3. 2010

Aljaž Merše Vičič
Mentor: doc. dr. Mitja Kožuh
Presoja in sprejetje sistemov ravnanja z okoljem po ISO 14001 v podjetju
Datum zagovora: 15. 7. 2010

Monika Mertik
Mentor: prof. dr. Marjan Bilban
Somentor: viš. pred. dr. Jožef Horvat
Odstranjevanje azbestne kritine
Datum zagovora: 22. 4. 2010

Nataša Mišković
Mentor: doc. dr. Mitja Kožuh
Identifikacija problemov hrupa v okolju s predlogi sanacije
Datum zagovora: 22. 10. 2010

Bojan Mohar
Mentor: prof. dr. Marjan Bilban
Mobbing na delovnem mestu
Datum zagovora: 15. 7. 2010

Staška Morela
Mentor: doc. dr. Mitja Kožuh
Gospodarjenje z odpadki v jeklarski industriji
Datum zagovora: 31. 3. 2010

Marko Ojsteršek
Mentor: pred. mag. Aleš Jug
Požarna varnost v termoelektrarni Šoštanj – javljanje požara s pomočjo video nadzornega sistema pri transportu premoga
Datum zagovora: 15. 7. 2010

Tomaž Omerzu
Mentor: doc. dr. Boris Jerman
Somentor: viš. pred. dr. Jože Šrekl
Varnost otrok v vrtcih in otroških igriščih
Datum zagovora: 17. 6. 2010

Jure Orličnik
Mentor: doc. dr. Mitja Kožuh
Energetska preskrba Slovenije – možnost uporabe obnovljivih virov
Datum zagovora: 7. 7. 2010

Tomaž Ožbold
Mentor: pred. mag. Aleš Jug
Umestitev objektov v urbano okolje
Datum zagovora: 23. 7. 2010

Mateja Pečjak
Mentor: doc. dr. Mitja Kožuh
Delovno okolje in varstvo pri delu v pralnici splošne bolnišnice
Datum zagovora: 23. 9. 2010

Franjo Podgoršek
Mentor: prof. dr. Marjan Bilban
Stres pri delu
Datum zagovora: 23. 9. 2010

Elvis Potočnik
Mentor: doc. dr. Mitja Kožuh
Obremenitev s hrupom v osnovni šoli Jožeta Moškriča
Datum zagovora: 22. 12. 2010

Valentina Robnik
Mentor: doc. dr. Mitja Kožuh
Primerjava kurišč na lesno biomaso s toplotnimi črpalkami
Datum zagovora: 23. 9. 2010

Boštjan Skopec
Mentor: pred. mag. Aleš Jug
Gašenje pnevmatik
Datum zagovora: 1. 2. 2010

Nikolaja Sorčan
Mentor: viš. pred. dr. Jože Šrekl
Somentor: Marjan Hrušovar, dr. med.
Strokovna izhodišča za oceno tveganja z vidika strokovnega sodelavca in medicine dela za livarja v podjetju Valji d.o.o. Štore
Datum zagovora: 22. 10. 2010

Klavdija Španbauer
Mentor: prof. dr. Marjan Bilban
Vplivi delovnega okolja na delazmožnost poklicnih voznikov
Datum zagovora: 15. 12. 2010

Miha Tavčar
Mentor: doc. dr. Boris Jerman
Varnost vrtnih kosilnic
Datum zagovora: 31. 8. 2010

Martin Trpin
Mentor: doc. dr. Mitja Kožuh
Somentor: viš. pred. dr. Jože Šrekl
Program za zmanjšanje poškodb pri delu v podjetju Hidria Rotomatika
Datum zagovora: 22. 4. 2010

Blaž Turk
Mentor: pred. mag. Aleš Jug
Določitev širine protipožarnih presek
Datum zagovora: 26. 5. 2010

Zoran Tuševski
Mentor: pred. mag. Aleš Jug
Program usposabljanja oseb odgovornih za gašenje začetnih požarov in izvajanje evakuacije
Datum zagovora: 26. 5. 2010

Mateja Zakrajšek
Mentorica: viš. pred. mag. Barbara Novosel
Novosti razvrščanja in označevanja kemikalij ter učinkovita prva pomoč pri brizgu jedke snovi
Datum zagovora: 28. 9. 2010

Jasmina Žakelj
Mentorica: prof. dr. Marija Bešter Rogač
Koncentracija prahu v livarni lahkih kovin
Datum zagovora: 1. 2. 2010

MAGISTERIJI

KEMIJA

Anuška Bole
Mentorica: prof. dr. Lucija Zupančič-Kralj
Vpliv emisij SO_2 na kislost padavin v okolici Šoštanja
Datum zagovora: 25. 3. 2010

KEMIJSKO INŽENIRSTVO

Boris Lisec
Mentorica: doc. dr. Ljudmila Fele Žilnik
Somentor: prof. dr. Janvit Golob
Izolacija lovastatina z ekstrakcijo tekoče – tekoče
Datum zagovora: 15. 12. 2010

UNIVERZITETNI PODIPLOMSKI ŠTUDIJ VARSTVA OKOLJA

Staša Kostevc
Mentor: prof. dr. Marjan Veber
Razvoj hitrega testa za ugotavljanje ustreznosti dezinfekcijskih sredstev in spremljanje njihovega vpliva v procesu biološkega čiščenja odpadnih vod
Datum zagovora: 29. 10. 2010

DOKTORATI

KEMIJA

Gregor Arh
Mentor: doc. dr. Matevž Pompe
Določevanje hlapnih organskih snovi pri neciljani analizi
Datum zagovora: 7. 5. 2010

Alan Bizjak
Mentor: prof. dr. Vojko Vlachy
Teoretične raziskave modelov vode in hidratacije ionskih in neionskih topljencev
Datum zagovora: 5. 5. 2010

Matjaž Bončina
Mentor: doc. dr. Jurij Reščič
Topnost lizocima v prisotnosti nevtralnega polimera in različnih elektrolitov
Datum zagovora: 13. 5. 2010

Bojan Burja
Mentor: prof. dr. Slovenko Polanc
Diazeni kot elektrofili v organski sintezi
Datum zagovora: 13. 10. 2010

Sanja Ćavar
Mentor: doc. dr. Franci Kovač
Oksidativne pretvorbe 4-metilkumarinov in njihovih derivatov
Datum zagovora: 15. 10. 2010

Viktor Drgan
Mentorica: doc. dr. Marjana Novič
Modeliranje retencijskih procesov in odnosov med kemijsko strukturo in retencijo v ionski kromatografiji
Datum zagovora: 20. 5. 2010

Matjaž Finšgar
Mentorica: znan. svet. dr. Ingrid Milošev
Somentor: prof. dr. Boris Pihlar
Benzotriazolni in polietileniminski inhibitorji korozije bakra in jekla v kloridnih raztopinah
Datum zagovora: 6. 12. 2010

Nina Hauptman
Mentorica: prof. dr. Marija Bešter Rogač
Somentorica: znan. sod. dr. Marta Klanjšek Gunde
Priprava in karakterizacija elektroprevodnih nanokompozitov
Datum zagovora: 15. 11. 2010

Mateja Hočevar
Mentorica: znan. sod. dr. Urša Opara Krašovec
Somentor: prof. dr. Boris Pihlar
Razvoj TiO_2 plasti za elektrokemijske sončne celice in ovrednotenje njihovega fotokatalitskega učinka
Datum zagovora: 31. 5. 2010

Jure Hren
Mentor: prof. dr. Marijan Kočevar
Sinteza in pretvorbe derivatov biciklo[2.2.2]oktenov in α,β-didehidro-α-aminokislin
Datum zagovora: 20. 4. 2010

Petra Igličar
Mentorica: prof. dr. Lucija Zupančič-Kralj
Določevanje razpadnih in metabolnih produktov inhibitorjev β-laktamaz
Datum zagovora: 26. 3. 2010

mag. Edita Jasiukaityte
Mentorica: prof. dr. Lucija Zupančič-Kralj
Somentor: doc. dr. Matjaž Kunaver
Identifikacija produktov kislinsko kataliziranega utekočinjenja celuloze in lignina z večfunkcionalnimi alkoholi
Datum zagovora: 13. 5. 2010

Špela Korent Urek
Mentorica: prof. dr. Aleksandra Lobnik
Somentor: prof. dr. Boris Pihlar
Razvoj novih optičnih kemijskih senzorjev za določevanje aminov in organofosfatov
Datum zagovora: 26. 11. 2010

Matjaž Koželj
Mentor: prof. dr. Boris Orel
Sinteza substituiranih trialkoksisilanov in njihova uporaba za pripravo materialov po sol-gel postopkih
Datum zagovora: 14. 5. 2010

Nika Lendero Krajnc
Mentor: doc. dr. Aleš Podgornik
Somentor: prof. dr. Boris Pihlar
Karakterizacija in optimizacija ionsko izmenjevalnih kromatografskih monolitov za izolacijo plazmidov
Datum zagovora: 29. 3. 2010

mag. Adrijana Leonardi
Mentor: prof. dr. Igor Križaj
Strukturna in biološka karakterizacija proteinskih komponent modrasovega strupa, ki vplivajo na proces strjevanja krvi
Datum zagovora: 6. 1. 2010

Miha Lukšič
Mentorica: prof. dr. Barbara Hribar Lee
Raziskave hidratacije polielektrolitov na primeru vodnih raztopin alifatskih ionenov
Datum zagovora: 13. 5. 2010

Mitja Martelanc
Mentor: prof. dr. Marijan Kočevar
Somentorica: viš. znan. sod. dr. Irena Vovk
Razvoj novih kromatografskih metod za določanje triterpenoidov v rastlinskih ekstraktih
Datum zagovora: 19. 11. 2010

Barbara Podobnik
Mentor: prof. dr. Radovan Komel
Funkcijska analiza citokroma P450 para-benzoatne hidroksilaze pri nitasti glivi *Cochliobolus lunatus*
Datum zagovora: 6. 12. 2010

Rebeka Toporišič
Mentor: prof. dr. Jurij Lah.
Raziskava stabilnosti enalaprilijevega maleata in termodinamika protolitskih ravnotežij te učinkovine v vodnih raztopinah
Datum zagovora: 13. 7. 2010

Vesna Weingerl
Mentor: prof. dr. Matija Strlič
Določanje fenolnih antioksidantov v vinu slovenskega porekla
Datum zagovora: 20. 12. 2010

Špela Župerl
Mentor: prof. dr. Jure Zupan
Somentorica: doc. dr. Marjana Novič
Kemometrijski pristop k iskanju povezav med kemijsko strukturo in lastnostjo učinkovin za njihovo načrtovanje in prenos v celice
Datum zagovora: 16. 3. 2010

KEMIJSKO INŽENIRSTVO

Petar Djinović
Mentor: prof. dr. Albin Pintar
Somentor: prof. dr. Janez Levec
Optimizacija CuO-CeO_2 mešanih oksidov kot katalizatorjev pri produkciji vodika iz plinske zmesi CO in vode ali etanola
Datum zagovora: 30. 6. 2010

Boštjan Klofutar
Mentor: prof. dr. Janvit Golob
Zagotavljanje stabilnosti dizelskega in biodizelskega goriva pri dolgoročnem hranjenju
Datum zagovora: 28. 1. 2010

MATERIALI

Marko Bitenc
Mentor: prof. dr. Stane Pejovnik
Somentorica: viš. znan. sod. dr. Zorica Crnjak Orel
Vpliv reakcijskih poti na morfologijo, rast in lastnosti delcev ZnO
Datum zagovora: 21. 6. 2010

Mirjana Küzma
Mentor: prof. dr. Janko Jamnik
Somentor: prof. dr. Stane Pejovnik
Elektrokemijsko ožičeni titanati za litij ionske baterije
Datum zagovora: 7. 5. 2010

RAZISKOVALNI PROGRAMIV LETU 2010
RESEARCH PROGRAMMES 2010

NOSILEC / PRINCIPAL RESEARCHER	**NASLOV** / TITLE
Prof. dr. Peter Bukovec	Bioanorganska in bioorganska kemija *Bioinorganic and bioorganic chemistry*
Prof. dr. Boris Pihlar	Raziskave in razvoj analiznih metod in postopkov *Research and development of analytical methods and procedures*
Prof. dr. Ivan Leban	Sinteza, struktura, lastnosti snovi in materialov *Synthesis, structure, properties of compounds and materials*
Akad. prof. dr. Branko Stanovnik	Sinteze in transformacije organskih spojin. Novi reagenti v stereoselektivni in regioselektivni sintezi aminokislin kot intermediatov v organski sintezi *Syntheses and transformations of organic compounds. New reagents in stereoselective and regioselective synthesis of amino acids as intermediates in organic synthesis*
Prof. dr. Vojeslav Vlachy	Fizikalna kemija *Physical chemistry*
Prof. dr. Marijan Kočevar	Organska kemija: sinteza, struktura, aplikacija *Organic chemistry: synthesis, structure and application*
Prof. dr. Matjaž Krajnc	Kemijsko inženirstvo *Chemical engineering*
Prof. dr. Janvit Golob	Separacijski procesi toplogrednih plinov za trajnostni razvoj *Separation processes of greenhouse gases for sustainable development*
Prof. dr. Dušan Turk*	Strukturna biologija *Structural biology*
Prof. dr. Igor Križaj*	Toksini in biomembrane *Toxins and biomembranes*
Izr. prof. ddr. Boris Turk*	Proteoliza in njena regulacija *Proteolysis and its regulation*
Akad. prof. dr. Janez Levec**	Kemijsko reakcijsko inženirstvo *Chemical reaction engineering*
Izr. prof. dr. Janez Plavec**	Kemija in struktura bioloških učinkovin *Chemistry and structure of biologically active compounds*
Izr. prof. dr. Albin Pintar**	Integralni pristop k preprečevanju onesnaževanja voda *Integrated approach to water pollution prevention*

* Institut »Jožef Stefan« / *Jožef Stefan Institute*

** Kemijski inštitut / *National Institute of Chemistry*

BIOANORGANSKA IN BIOORGANSKA KEMIJA
BIOINORGANIC AND BIOORGANIC CHEMISTRY

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0134

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Peter Bukovec

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
prof. dr. Nataša Bukovec
prof. dr. Peter Bukovec
prof. dr. Marko Zupan
dr. Sabina Grabner
doc. dr. Barbara Modec
dr. Elizabeta Tratar Pirc
doc. dr. Romana Cerc Korošec
doc. dr. Marija Zupančič
doc. dr. Marjan Jereb
dr. Irena Kozjek Škofic
Nataša Čelan Korošin, univ. dipl. kem

Mladi raziskovalci / Young Researchers
Jerneja Šauta Ogorevc
Ksenija Cer Kerčmar

Tehniki / Technicians
Damjan Erčulj
Urška Levec

Sodelujoče institucije / Participating Institutions
Institut Jožef Stefan

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Modelne spojine v bioanorganski in bioorganski kemiji, sinteze novih organskih in anorganskih spojin z biološko aktivnostjo, antioksidanti, kovinske spojine v okolju in njihova imobilizacija, razvoj novih sintetskih metod, študij mehanizmov halogeniranja.

OSREDNJE TEME PROGRAMA

Kemija molibdenovih klastrov, bioaktivni kompleksi, kovine v okolju, emulzije in zelena kemija, jodiranje z elementarnim jodom, nove metode halogeniranja.

ZNANSTVENI DOSEŽKI

BIOANORGANSKI SKLOP

V nadaljevanju naših raziskav o večjedrnih okso koordinacijskih spojinah molibdena(V) smo določili kristalni strukturi dveh spojin, ki vsebujeta prototip dvojedrne $\{Mo_2O_4\}^{2+}$ enote: $[Mo_2O_4Cl_2Py_4]\cdot 2.25Py$ in $[Mo_2O_4Cl_2Py_4]\cdot 1.5PyHCl$. Obe nastaneta pri reakciji enojedrnih ionov $[MoOCl_4(H_2O)]^-$ s piridinom. Velika vsebnost slednjega v reakcijski zmesi prepreči nadaljnjo agregacijo dvojedrnih enot v večje klastre. Dobljene rezultate smo publicirali v online reviji Materials (MODEC, Barbara, ZUBIETA, Jon. Syntheses and a solid state structure of a dinuclear molybdenum(V) complex with pyridine. Materials 3 (2010) 150–157). Dosedanje delo na področju omenjenih spojin je maja 2010 Barbara Modec predstavila na vabljenem predavanju na Universität des Saarlandes v Saarbrücknu v Nemčiji. Naslov predavanja je bil »Overview of polyoxomolybdates: chemistry, structures and applications«.

V letu 2010 so bile naše raziskave usmerjene na pojasnjevanje delovanja naravnega antioksidanta ksanturinske kisline (Xan) v naravnem okolju, kjer je prisotna tudi vrsta kovinskih ionov. S tem namenom smo sintetizirali in karakterizirali vrsto koordinacijskih spojin s kovinskimi ioni Cu^{2+}, Pd^{2+}, Cd^{2+}. Preučevali smo tudi antioksidativne lastnosti raztopin same izhodne spojine Xan in z njo pripravljenih kompleksov ter polimorfizem Xan. Pripravili smo dve bakrovi koordinacijski spojini s sestavo $[Cu(Xan)(H_2O)_2]$ in $[Cu(Xan)(H_2O)_2]\ H_2O$, ki predstavljata isti kompleks, s tem, da eden vsebuje solvatno vodo, drugi pa ne. Delne rezultate smo predstavili na konferenci (CER KERČMAR, Ksenija, TRATAR PIRC, Elizabeta, MODEC, Barbara, BUKOVEC, Peter. Sinteza in karakterizacija bakrovega(II) kompleksa s ksanturinsko kislino = Synthesis and characterization of copper(II) complex with xanthurenic acid. V: Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010. [Maribor]: FKKT, [2010], str. 1–10). S paladijevimi(II) ioni smo sintetizirali dva popolnoma različna kompleksa $[PdXan(H_2O)]$ in $[Pd_2(Xan)_2(DMSO)_2]\cdot 2DMSO$, v odvisnosti od uporabljenega topila in načina priprave. Določili pa smo tudi kristalno strukturo dvojedrne kadmijeve(II) spojine $[Cd_2(Xan)_2(H_2O)_4]$.

Na področju raziskav anaerobne razgradnje z OxiTop metodo smo nadaljevali s proučevanjem inhibitornega delovanja cianidov na proces razgradnje. Objavljen je bil članek (TRATAR PIRC, Elizabeta, LEVSTEK, Meta, BUKOVEC, Peter. Influence of cyanide on the anaerobic degradation of glucose. Water sci. technol., 2010, vol. 62, no. 8, str. 1799–1806).

Kurkumin je hidrofoben polifenol z visokim antioksidativnim potencialom in je obetajoč terapevtik za več bolezni. Glavna ovira, ki omejuje njegovo uporabo v medicini, je njegova nizka biološka razpoložljivost. Da bi povečali prenos kurkumina v organe in tkivo, smo poskusili pripraviti njegove derivate, ki bi bili vodotopni. Osredotočili smo se na sinteze derivatov, s katerimi bi vezali hidrofilno skupino npr. glukoronsko kislino na kurkumin. Pri pripravi vodotopnega derivata kurkumina smo tudi poskušali vezati nabito amino skupino na alkilno verigo, ki leži na nasprotni strani hidroksilne fenolne skupine. Prav tako smo poskusili že sintetizirane derivate inkorporirati v γ-cyclodextrin.

S pomočjo termogravimetrije in diferenčne dinamične kalorimetrije tankih plasti $Bi_{12}SiO_{20}$ smo določili začetno temperaturo toplotno obdelave tega keramičnega dielektričnega materiala (250 °C), da pri nadaljnjem segrevanju do 700 °C ni prišlo do pokanja in je bila končna struktura gosta in homogena (VEBER, Asja, KUNEJ, Špela, CERC KOROŠEC, Romana, SUVOROV, Danilo. The effects of solvents on the formation of sol-gel-derived $Bi_{12}SiO_{20}$ thin films. J. Eur. Ceram. Soc., 2010, vol. 30, no. 12, str. 2475–2480). Z metodami termične analize smo poskušali dokazati, da se elektroaktivne organske molekule vežejo na površino nanodelcev SiO_2, kar vodi do odlične elektrokemijske stabilnosti organsko-anorganskega sistema (GENORIO, Boštjan, PIRNAT, Klemen, CERC KOROŠEC, Romana, DOMINKO, Robert, GABERŠČEK, Miran. Electroactive organic molecules immobilized onto solid nanoparticles as a cathode material for lithium-ion batteries. Angew. Chem. (Int. ed., Print)., 2010, vol. 49, no. 40, str. 7222–7224).

Nadaljevali smo z raziskovanjem CeO_2 ionskih hranilnikov, pripravljenih po sol-gel postopku. V CeO_2 sol smo dodajali vanadij v različnih razmerjih. Z ciklovoltametrijo (CV), kronokulometrijo (CPC) in merjenjem različnih optičnih lastnosti smo preverjali ustreznost lastnosti pripravljenih tankih plasti mešanih oksidov Ce in V. V sodelovanju z Univerzo v Mariboru smo izvedli meritve podaljšane fine strukture rentgenskih robov (EXAFS), (KOZJEK ŠKOFIC, Irena, PADEŽNIK GOMILŠEK, Jana, KODRE, Alojz, BUKOVEC, Nataša. Electrochemical, optical and X-ray absorption studies of Ce/V mixed oxides thin films. Sol. energy mater. sol. cells. [Print ed.], 2010, vol. 94, no. 3, str. 554–559).

V letu 2010 smo se ukvarjali z optimizacijo fotokatalitske celice (optimizacija razmerja med prostornino raztopine in površino tankih plasti), s katero je v fotoreaktorju mogoče oceniti fotokatalitsko učinkovitost pripravljenih tankih plasti. Uspešno so bili sintetizirani soli in pripravljene tanke plasti iz prekurzorja $TiOSO_4$. Fotokatalitska aktivnost je bila ocenjena za vse do sedaj pripravljene tanke plasti, pri čemer smo kot vir svetlobe uporabili ne samo UVA žarnic temveč tudi žarnice, ki simulirajo dnevno svetlobo. Iz $TiCl_4$ prekurzorja smo pripravili tudi dopirane tanke plasti (z zlatom, srebrom in železom), med katerimi so najbolj fotokatalitsko aktivne plasti dopirane z zlatom. Preverili smo tudi protimikrobno delovanje dopiranih tankih plasti pod vidno svetlobo. Z mikroskopom na atomsko silo je bila ocenjena hrapavost vseh pripravljenih plasti. Solom smo dodajali surfaktant Pluronic F127, ki je povečal fotokatalitsko aktivnost, saj so takšne plasti bolj porozne. Sodelovanje smo razširili s Katedro za kemijsko, biokemijsko in ekološko inženirstvo, FKKT, kjer opravljamo toksikološke študije.

V letu 2010 smo nadaljevali z raziskavami kemijske stabilizacije kovin v onesnaženih tleh. Na osnovi naših izkušenj z uporabo fosfatnih vezalcev smo naše raziskave razširili na uporabo kombiniranih vezalcev (fosfati in apno). Izvedli smo obširno raziskavo (del raziskave je še vedno v teku) z uporabo onesnaženih tal s področja stare Cinkarne v Celju. Delne rezultate raziskav smo predstavili na dveh mednarodnih konferencah (ZUPANČIČ, Marija, CENCELJ, Jure, BUKOVEC, Peter. Evaluation of the use of phosphate stabilisation agents for metal contaminated soils. Protection and Restoration of the Environment X, 5–9 July 2010, Corfu,

Greece; ZUPANČIČ, Marija, BUKOVEC, Peter. Evaluation of the metal stabilization efficiency and drawbacks of phosphate treatment of contaminated soil. Proceedings of the 15th International Conference on Heavy Metals in the Environment, September 19–23, 2010, Gdańsk, Poland).

BIOORGANSKI SKLOP

V okviru bioorganskega dela programa smo nadaljevali raziskave na področju transformacij, s poudarkom na halogeniranju organskih spojin pod okolju prijaznejšimi reakcijskimi pogoji. Odkrili in razvili smo metodo direktnega fluoriranja 1,3-dikarbonilnih spojin v vodnem mediju z uporabo reagenta Selectfluor™ F-TEDA-BF_4 in z uporabo reagenta Accufluor™ NFSi pod reakcijskimi pogoji brez uporabe topil (RPBUT). V obeh primerih smo ciklične 1,3-dikarbonilne derivate pretvorili v 2-fluoro substituirane produkte, aciklične analoge pa v 2,2-difluoro produkte. Fluoriranje 1-trifluorometil derivatiziranih 1-3-dikarbonilnih derivatov je poteklo do 2,2-difluoro-3,3-dihidroksi-1-onov. Dokazali smo, da je reaktivnost substratov v vodnem mediju odvisna od njihove enolizabilnosti, hidrofilnosti in agregatnega stanja pri reakcijski temperaturi. Reakcije pod RPBUT so potekale v talini pri evtektični temperaturi. Izmerili smo tudi faktorje relativne hitrosti za te transformacije. Prvi smo pokazali, da je mogoče pod RPBUT direktno fluorirati tudi ketone in vse te rezultate objavili v vodilni reviji s področja aplikativne kemije Advanced Synthesis&Catalysis. Odkrili in razvili smo novo metodo za aerobne oksidativne transformacije organskih spojin z uporabo reakcijskega sistema zrak/HNO_3(cat)/ TEMPO (cat) in odkritje aplicirali na selektivno oksidacijo alkoholov do aldehidov ali ketonov in oksidativno jodiranje organskih spojin z elementarnim jodom. Razvili smo metodo priprave ariljodo(III)dikloridov s postopkom oksidativnega kloriranja s sistemom HCl(35 %)/ H_2O_2(30 %) v trifluoroetanolu, ki ima vlogo topila in aktivatorja vodikovega peroksida in ugotovili, da imajo elektron-donor substituente na aromatskem jedru, sicer pozitiven vpliv na potek reakcije, toda produkti so nestabilni, reakcija nadalje poteče do tvorbe kloriranih aromatov. Na povabilo uredništva smo pripravili prispevek za ugledno enciklopedično publikacijo Encyclopedia of Reagents for Organic Synthesis.

Za terciarne benzilne alkohole je znano, da jih s F-TEDA-BF_4 v acetonitrilu lahko pretvorimo v ustrezne β-fluoro hidrinske derivate. Reakcijski medij je pogosto zdravju škodljivo hlapno organsko topilo, ki ga želimo nadomestiti z bolj prijaznim reakcijskim medijem. Kot topilo bi bila voda v tem pogledu najboljši reakcijski medij, vendar omejitve često predstavlja slaba topnost organskih spojin. Tako smo kot reakcijski medij testirali vodno raztopino surfaktanta, ki tvori micele. Študirali smo vpliv koncentracije posameznega surfaktanta na pretvorbo 1,1-difeniletanola s F-TEDA-BF_4 in ugotovili, da natrijev dodecil sulfat (NaDS) in dodecil benzensulfonska kislina (DBSK) močno pospešita nastajanje 1,1-difenil-2-fluoroetanola. Serijo modelnih terciarnih benzilnih alkoholov smo s F-TEDA-BF_4 v raztopinah obeh amfifilov pri 85 °C uspešno pretvorili v β-fluoro hidrine. Sterično bolj ovirani substrati (npr. 1,1,2-trifeniletanol) so manj reaktivni (reak. čas = 15 h), medtem ko 1,1-difeniletanol popolnoma zreagira v dveh urah v raztopini NaDS. Z namenom, da bi dobili kar največ informacij o mehanističnem poteku pretvorbe, smo sintetizirali več strukturno različnih terciarnih alkoholov, ki jih testiramo pod omenjenimi pogoji. Del teh rezultatov je bil predstavljen na 16. evropskem simpoziju o kemiji fluora v Ljubljani 2010.

Ionske tekočine so obnovljiv reakcijski medij, ki ga lahko večkrat zaporedoma uporabimo za pretvorbe organskih spojin. 1-Metil-3-(sulfobutil)imidazolijev triflat oz. [BMIM(SO_3H)] [OTf], ki ima lastnosti Brønstedove kisline smo uporabili kot reakcijski medij za transformacijo organskih molekul z NXS reagenti. Transformacije aromatskih ketonov z NIS regiose-

lektivno vodijo do nastanka α-jodiranih ketonov. Pretvorbe z NBS so manj selektivne; poleg bromiranja na α-mestu, v primeru močno aktiviranega aromatskega jedra z dvema metoksi skupinama, poteče tudi bromiranje obroča. Podobno reaktivnost smo opazili tudi v primeru NCS. Pretvorbe nekaterih aktiviranih aromatov vodijo do o- in p-halogeniranih produktov. Pretvorbe substratov z dvema ekvivalentoma NXS vodijo do nastanka dihalogeniranih produktov. To ionsko tekočino lahko uporabimo večkrat, njena učinkovitost pa je bila tudi po desetih ciklih nespremenjena. Del rezultatov je bil predstavljen na posvetovanju Slovenski kemijski dnevi 2010 v Mariboru.

Prispevki so bili publicirani v:

– STAVBER, Gaj, STAVBER, Stojan. Towards greener fluorine organic chemistry : Direct electrophilic fluorination of carbonyl compounds in water and under solvent-free reaction conditions. Advanced Synthesis & Catalysis. [Print ed.], 2010, vol. 352, no. 16, str. 2838–3846.
– PODGORŠEK, Ajda, ISKRA, Jernej. Conversion of aryl iodides into aryliodine(III) dichlorides by an oxidative halogenation strategy using 30% aqueous hydrogen peroxide in fluorinated alcohol. Molecules (Basel), 2010, vol. 15, no. 4, str. 2857–2871.

In predstavljeni na konferencah:

– VRAŽIČ, Dejan, JEREB, Marjan, STAVBER, Stojan, LAALI, Kenneth K. Halogeniranje organskih spojin z NXS reagenti v ionskih tekočinah = Halogenation of organic compounds in ionic liquids using NXS reagents. V: Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010.
– VRAŽIČ, Dejan, STAVBER, Gaj, JEREB, Marjan, STAVBER, Stojan. Micellar system-mediated direct conversion of tert. alcohols to vicinal fluorohydrins in water using SELECTFLUOR[sup](TM) D-TEDA-BF[sub]4. V: SKAPIN, Tomaž (ur.). 16th European Symposium on Fluorine Chemistry – ESFC, July 18–23, 2010, Ljubljana, Slovenia. [Book of abstracts]. Ljubljana: Jožef Stefan Institute, 2010, str. 345.
– ŽMITEK, Katja, PODGORŠEK, Ajda, ISKRA, Jernej. Fluorinated alcohol as media for electrophilic and acid-catalyzed reactions. V: SKAPIN, Tomaž (ur.). 16th European Symposium on Fluorine Chemistry – ESFC, July 18–23, 2010, Ljubljana, Slovenia. [Book of abstracts]. Ljubljana: Jožef Stefan Institute, 2010, str. 321.

DRUGI RELEVANTNI DOSEŽKI

Nekateri člani programske skupine so vključeni v centre odličnosti: CO NOT – Center odličnosti: Nizkoogljične tehnologije: Peter Bukovec, Nataša Bukovec, Irena Kozjek Škofic, Damjan Erčulj. CO ENFIST – Center odličnosti: Raziskave na področju zdravja, znanosti o življenju in naprednih novih materialov: Peter Bukovec, Elizabeta Tratar Pirc.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

Model compounds in bioinorganic and bioorganic chemistry, synthesis of new organic and inorganic compounds with biological activity, antioxidants, metal compounds in the environment and their immobilization, new synthetic methods, mechanisms of halogenation.

RESEARCH TOPICS

Chemistry of molybdenum clusters, bioactive metal complexes, metals in the environment, emulsions and green chemistry, iodination with elemental iodine, new methods of halogenation.

SCIENTIFIC ACHIEVEMENTS

BIOINORGANIC CHEMISTRY

As part of our ongoing research on oxomolybdenum(V) polynuclear species, we determined X-ray structures of two compounds containing a prototype of a dinuclear $\{Mo_2O_4\}^{2+}$ unit: $[Mo_2O_4Cl_2Py_4]\cdot 2.25Py$ and $[Mo_2O_4Cl_2Py_4]\cdot 1.5PyHCl$. Both were isolated from the reaction of the mononuclear $[MoOCl_4(H_2O)]^-$ ion with pyridine. A high content of pyridine in the reaction mixture prevents further aggregation of dinuclear cores into larger clusters (MODEC, Barbara, ZUBIETA, Jon. Syntheses and a solid state structure of a dinuclear molybdenum(V) complex with pyridine. Materials 3 (2010) 150–157). The results of our work in the field of polyoxomolybdate chemistry were presented by Barbara Modec in her lecture »Overview of polyoxomolybdates: chemistry, structures and applications« at the Universität des Saarlandes in Saarbrücken in Germany in May 2010.

Our research has been focused on explaining the function of the natural antioxidant xanthurenic acid (Xan) with series of metal ions in a natural environment. A series of coordination compounds with metal ions of Cu^{2+}, Pd^{2+}, Cd^{2+} were synthesized and characterized. The antioxidant properties of the solutions of Xan and its complexes were investigated and polymorphism of Xan were studied. Two copper compounds $[Cu(Xan)(H_2O)_2]$ and $[Cu(Xan)(H_2O)_2]\cdot H2O$ were prepared. Both compounds consist of neutral complex molecules with the $[Cu(Xan)(H_2O)_2]$ composition. Compound $[Cu\ (Xan)(H_2O)_2]\cdot H_2O$ also contains a water molecule of crystallization, one per formula unit. Partial results were presented at the conference (CER KERČMAR, Ksenija, TRATAR PIRC, Elizabeta, MODEC, Barbara, BUKOVEC, Peter. Synthesis and characterization of copper(II) complexes with xanturinic acid: Slovenian Chemical Days 2010, Maribor, 23 and 24 September 2010th [Maribor]: FKKT, [2010] page 1–10). Two fundamentally different types of complexes with palladium(II) ions $[PdXan(H_2O)]$ and $[Pd_2(Xan)_2(DMSO)_2]\cdot 2DMSO$ were synthesized, depending on the solvent used and the method of preparation. The crystal structure of binuclear cadmium(II) compounds $[Cd_2(Xan)_2(H_2O)_4]$ was also determined.

The research of inhibitory effects of cyanides on anaerobic degradation of glucose, using the OxiTop method has been continued. The results of our study were published (TRATAR PIRC, Elizabeta, LEVSTEK, Meta, BUKOVEC, Peter. Influence of cyanide on the anaerobic degradation of glucose. Water sci. technol., 2010, Vol. 62, no. 8, p.p. 1799–1806).

Curcumine is a hydrophobic polyphenol with high antioxidative potential and is a promising therapeutic for several diseases. The major hindrance limiting its exploitation in medicine is its low bioavailability. To enhance curcumine delivery into organs and tissues we tried to prepare its derivatives which would be soluble in water. We focused on the preparation of curcumine derivatives by attaching hydrophilic groups, for example glucuronic acid. In the preparation of water-soluble derivative of curcumin, we also tried to modify its structure by binding a charged amino group to the alkyl chain which lies on the opposite side of the phenolic hydroxyl group. At the same time we were also seeking how to solubilize previously prepared new derivatives of curcumine with the incorporation into γ-cyclodextrin.

Following the results of of thermogravimetric measurements and dynamic scanning calorimetry of $Bi_{12}SiO_{20}$ thin films, a pre-heating temparature of 250 °C was determined. During additional thermal tratement up to 700 °C, cracks were not formed within this ceramic dielectric material, leading to dense and homogeneous final structure. (VEBER, Asja, KUNEJ, Špela, CERC KOROŠEC, Romana, SUVOROV, Danilo. The effects of solvents on the formation of sol-gel-derived $Bi_{12}SiO_{20}$ thin films. J. Eur. Ceram. Soc., 2010, Vol. 30, No. 12, p.p. 2475–2480). By applying thermal methods we tried to prove that electroactive organic molecules bind onto silica nanoparticles, leading to excellent electrochemical stability of organic-inorganic hybrid system (GENORIO, Boštjan, PIRNAT, Klemen, CERC KOROŠEC, Romana, DOMINKO, Robert, GABERŠČEK, Miran. Electroactive organic molecules immobilized onto solid nanoparticles as a cathode material for lithium-ion batteries. Angew. Chem. (Int. ed., Print)., 2010, Vol. 49, No. 40, p.p. 7222–7224).

We have continued studying CeO_2 ion-storage films prepared by sol-gel method. Mixed oxides of Ce and V were prepared in various ratios. Cyclovoltametry (CV), chronocoulometry (CPC) and different optic methods were used to determine properties of thin films. In collaboration with the Faculty of Mechanical Engineering in Maribor we performed measurements of Extended X-ray Absorption Fine Structure (EXAFS) of the prepared thin films. The work was published (KOZJEK-ŠKOFIC, Irena, PADEŽNIK GOMILŠEK, Jana, KODRE, Alojz, BUKOVEC, Nataša. Electrochemical, optical and X-ray absorption studies of Ce/V mixed oxides thin films. Sol. energy mater. sol. cells. [Print ed.], 2010, Vol. 94, No. 3, p.p. 554–559).

In 2010, we also focused our research on the optimisation of the photocatalytic cell (optimization of ratio between the volume of the solution and photocatalyst's surface area) which was used to estimate photocatalytic activity of the prepared thin films. Synthesis of sol from $TiOSO_4$ precursor was successfully developed and thin films were tested for photocatalytic activity under UVA and visible light. From sols made from $TiCl_4$, the precursor-doped thin films were prepared (Au, Ag and Fe) of which Au-doped thin films were the most active. All films were tested for antibacterial activity. Surfactant Pluronic F127 was added into the sol to enhance photocatalytic activity. In cooperation with the Chair of Chemical, Biochemical and Environmental Engineering at our Faculty were performed toxicity studies.

In 2010, we continued our research work on chemical stabilization of metals in contaminated soil. According to our previous results with phosphate stabilization agents, an extensive study has been carried out (which is still going on), dealing with combined stabilization agents (phosphate and lime) and heavily contaminated soil from the Celje region. Partial results of our study were presented at two international conferences (ZUPANČIČ, Marija, CENCELJ, Jure, BUKOVEC, Peter. Evaluation of the use of phosphate stabilisation agents for metal contaminated soils. Protection and Restoration of the Environment X, 5–9 July 2010, Corfu, Greece; ZUPANČIČ, Marija, BUKOVEC, Peter. Evaluation of the metal stabilization efficiency and drawbacks of phosphate treatment of contaminated soil. Proceedings of the 15th International Conference on Heavy Metals in the Environment, September 19–23, 2010, Gdańsk, Poland).

BIOORGANIC CHEMISTRY

Within the framework of bioorganic part of the programme we continued the investigation on the application of principles of green chemistry in transformations of organic compounds, stressing the selective introduction of halogen atoms into organic compounds. Selective and efficient fluorination of organic 1,3-dicarbonyl compounds was achieved by using the electrophilic fluorinating reagents Selectfluor™ F-TEDA-BF_4 (1-chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis tetrafluoroborate) in aqueous medium or Accufluor™ NFSi (N-fluorobenzensulfonimide) under solvent-free reaction conditions (SFRC). Under both reaction conditions cyclic 1,3-dicarbonyl compounds were transformed into 2-fluoro substituted derivatives and acyclic analogues into 2,2-difluoro substituted compounds, while the reactions of 1-trifluoromethyl substituted 1,3-dicarbonyls in water resulted in the formation of 2,2-difluoro-3,3-dihydroxy-1-one derivatives. The reactivity of the starting material in water was found to be dependent on its enolizability, hydrophobic interactions and aggregate state at the reaction temperature. Reactions under SFRC proceeded in the molten eutectic phase of the reactants. The technique of competitive reactivity was used in order to evaluate and better understand the effects of reaction conditions on the course of these reactions. We originally showed that direct fluorination of ketones could be performed also under SFRC. We published our findings in Advanced Synthesis&Catalysis, which is the leading journal for applied chemistry.

We discovered and developed a new method for aerobic oxidative transformation of organic compounds, using the reaction system air/HNO_3(cat)/TEMPO (cat) and applied the method for oxidation of alcohols to aldehydes or ketones and oxidative iodination of organic compounds using elemental iodine. Oxidative chlorination with HCl/H_2O_2 in 1,1,1-trifluoroethanol was used to transform aryl iodides into aryliodine(III) dihalides. In this particular case 1,1,1-trifluoroethanol is not only the reaction medium, but also an activator of hydrogen peroxide for the oxidation of hydrochloric acid to molecular chlorine. Aryliodine(III) dichlorides were formed in 72–91% isolated yields in the reaction of aryl iodides with 30% aqueous hydrogen peroxide and hydrochloric acid at ambient temperature. A study on the effects which the substituents on the aromatic ring have on the formation and stability of aryliodine(III) dichlorides showed that the transformation is easier to achieve in the presence of the electron-donating groups (i.e. methoxy), but in this case the products rapidly decompose under the reported reaction conditions to form chlorinated arenes. Our group was invited to prepare the contribution for Encyclopedia of Reagents for Organic Synthesis.

It is known that the transformation of tertiary benzylic alcohols with F-TEDA-BF_4 in acetonitrile produced the corresponding β-fluorohydrins. The reaction medium is often a volatile organic solvent, harmful to health, and for this reason we would like to find a more friendly replacement for it. Water is considered to be the best solvent in this regard, however poor solubility of organic compounds often represents limitation for its use. As a reaction medium we have tested aqueous solution of surfactant which forms micelles. We studied the role of concentration of each of surfactants on conversion of 1,1-diphenylethanol with F-TEDA-BF_4 to find that sodium dodecyl sulfate (SDS) and dodecyl benzenesulfonic acid (DBSA) significantly accelerated the formation of 1,1-diphenyl-2-fluoroethanol. A series of model tertiary benzylic alcohols was successfully transformed with F-TEDA-BF_4 at 85°C to β-fluorohydrins in solutions of both surfactants. Sterically more hindered substrates (for example, 1,1,2-triphenylethanol) were less reactive (react. time = 15h), while 1,1-diphenylethanol fully reacted in a solution of SDS within two hours. In order to get a deeper insight into the mechanistic pathway, we synthesized a series of structurally different tertiary alcohols, and their testing under the above mentioned conditions is currently underway. A part of these results was presented at the 16th European Symposium on Fluorine Chemistry in Ljubljana. in 2010.

Ionic liquids represent recyclable reaction medium which can be used consecutively for several times for the transformation of organic molecules. As a reaction medium for the transformation of organic molecules with NXS reagents we used 1-methyl-3-(sulfobutyl)imidazolium triflate or [BMIM(SO_3H)][OTf] which possess Brønsted acid properties. Functionalization of aromatic ketones with NIS regioselectively produced α-iodo ketones. Transformations with NBS were less selective; besides α-bromo ketones, in case of strongly activated aromatic ring with two methoxy groups, bromination of the aromatic ring took place as well. NCS exhibited similar reactivity. Transformations of activated aromatics furnished o- and p- halogenated products. Functionalization of substrates with two equivalents of NXS led to the formation of dihalogenated products. This ionic liquid could be reused several times, its efficiency remained unchanged even after ten cycles. A part of these results was presented at the Slovenski kemijski dnevi conference 2010 in Maribor.

Scientific results were published in:

– STAVBER, Gaj, STAVBER, Stojan. Towards greener fluorine organic chemistry : direct electrophilic fluorination of carbonyl compounds in water and under solvent-free reaction conditions. Advanced Synthesis & Catalysis. [Print ed.], 2010, Vol. 352, No. 16, p.p. 2838–3846.
– PODGORŠEK, Ajda, ISKRA, Jernej. Conversion of aryl iodides into aryliodine(III) dichlorides by an oxidative halogenation strategy using 30% aqueous hydrogen peroxide in fluorinated alcohol. Molecules (Basel), 2010, Vol. 15, No. 4, p.p. 2857–2871.

And presented at conferences:

– VRAŽIČ, Dejan, JEREB, Marjan, STAVBER, Stojan, LAALI, Kenneth K. Halogeniranje organskih spojin z NXS reagenti v ionskih tekočinah = Halogenation of organic compounds in ionic liquids using NXS reagents. V: Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010.
– VRAŽIČ, Dejan, STAVBER, Gaj, JEREB, Marjan, STAVBER, Stojan. Micellar system-mediated direct conversion of tert. alcohols to vicinal fluorohydrins in water using SELECTFLUOR[sup](TM) D-TEDA-BF[sub]4. V: SKAPIN, Tomaž (ur.). 16th European Symposium on Fluorine Chemistry – ESFC, July 18–23, 2010, Ljubljana, Slovenia. [Book of abstracts]. Ljubljana: Jožef Stefan Institute, 2010, p. 345.
– ŽMITEK, Katja, PODGORŠEK, Ajda, ISKRA, Jernej. Fluorinated alcohol as media for electrophilic and acid-catalyzed reactions. V: SKAPIN, Tomaž (ur.). 16th European Symposium on Fluorine Chemistry – ESFC, July 18–23, 2010, Ljubljana, Slovenia. [Book of abstracts]. Ljubljana: Jožef Stefan Institute, 2010, p. 321.

OTHER RELEVANT ACHIEVEMENTS

Some members of the programme group have been active in two Centers of Excellence:

CO NOT – Center of Excellence: Low Carbon Technologies: Peter Bukovec, Nataša Bukovec, Irena Kozjek Škofic, Damjan Erčulj. CO ENFIST – Center of Excellence: Multidisciplinary Research in Life Sciences and Advanced New Materials: Peter Bukovec, Elizabeta Tratar Pirc.

RAZISKAVE IN RAZVOJ ANALIZNIH METOD IN POSTOPKOV
RESEARCH AND DEVELOPMENT OF ANALYTICAL METHODS AND PROCEDURES

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0153

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Boris Pihlar

SODELAVCI PROGRAMSKE SKUPINE / PROGRAMME GROUP CO-WORKERS

Raziskovalci / Researchers
prof. dr. Boris Pihlar
prof. dr. Marjan Veber
izr. prof. dr. Lucija Zupančič-Kralj
izr. prof. dr. Nataša Gros
izr. prof. dr. Matija Strlič
doc. dr. Helena Prosen
doc. dr. Matevž Pompe
doc. dr. Drago Kočar
dr. Robert Susič
dr. Tatjana Zupančič
doc. dr. Irena Kralj Cigić
dr. Polonca Kralj
dr. Martin Šala

Mladi raziskovalci / Young Researchers
Gregor Arh
Tanja Trafela
Andrej Ščavničar
Alenka Možir

Tehniki / Technicians
Ivanka Keber
Zdenka Držaj
Jolanda Furlan
Mojca Žitko

POROČILO O REALIZACIJI PROGRAMA

CILJI IN OSREDNJE TEME PROGRAMA

Med osnovne cilje programa spadajo:

a) temeljne raziskave analiznih metod in pristopov,
b) raziskave in razvoj metod za analizo in karakterizacijo materialov,
c) razvoj metod in postopkov za kontrolo kakovosti v industriji, varnosti živil in okolju.

ZNANSTVENI IN DRUGI RELEVANTNI DOSEŽKI

Sodelavci programske skupine so v letu 2010 objavili 30 izvirnih znanstvenih člankov (Bibliografija katedre za analizno kemijo, AL1-AL30) in dva kratka znanstvena prispevka (AL31-AL32), imeli eno vabljeno predavanje (AL33) in 11 znanstvenih prispevkov na konferencah (AL34-AL44) ter pridobili en evropski patent (Al49).

Raziskovali smo naslednje:

a)

Za karakterizacijo katalizatorjev, ki se uporabljajo v gorivnih celicah, smo uporabili mikroelektrodo iz ogljikovega mikrovlakna (AL17). S posebno pripravo smo dobili ustrezen kompakten nanos katalizatorja na mikroelektrodo, ki je omogočal spremljanje adsorbcijsko–desorpcijskih procesov in študij kinetike elektrokemijske redukcije kisika. Pomembna prednost mikroelektrode je enostavna in hitra priprava, ki skrajša čas meritve in karakterizacije katalizatorja na 5–10 minut.

V članku objavljenem v reviji Electroanalysis (AL28) smo titanatne nanocevke (TiNT) modificirali z »Berlinsko modrim« (BM), ki smo ga sintetizirali z reakcijo med heksacianoferatom(III) nanešenim na TiNT in Fe(II) ioni. BM–TiNT modificirane nanocevke katalizirajo redukcijo vodikovega peroksida, konstanta hitrosti pa je za red velikosti višja od klasično elektrokemijsko pripravljenih tankih plasti BM. Ugotovili smo, da modifikacija z manj kot nanomolarno plastjo BM, zagotavlja stabilen in ponovljiv odziv na H_2O_2 v območju med 0,02 in 0,4 mM in omogoča določanje peroksida pri nizkih napetostih (–0,15 V).

Izpeljali smo splošno metodologijo za ovrednotenje negotovosti za ione v kombiniranih kalibracijskih standardnih raztopinah (AL3), kjer se koncentracije lahko razlikujejo tudi do pet redov velikosti, in sicer z namenom, da bi prepoznali glavne prispevke k negotovosti. Dokazali smo, da je utemeljeno upoštevati navzkrižno kontaminacijo, podobno kot je že uveljavljena

praksa, da se upošteva stopnjo čistosti kemikalij, saj imajo nečistoče lahko signifikanten vpliv na negotovost koncentracije iona že, če je koncentracija iona, ki vnaša nečistočo, petindvajsetkrat višja od koncentracije iona, na katero nečistoča vpliva. Dokazali smo, da je za masno koncentracijo mnogih ionov to glavni vir negotovosti.

Članek objavljen v reviji Analytica Letters (AL4**)** kritično obravnava prispevke k merilni negotovosti pri simultanem določanju makro in mikro komponent v morski vodi in sorodnih raztopinah z ionsko kromatografijo in uporabo kombiniranih kalibracijskih standardov, kjer prihaja do problema navzkrižne kontaminacije. Negotovost pri določitvi koncentracij kationov in anionov smo soočili z negotovostmi njihovih koncentracij v kombiniranih kalibracijskih raztopinah. Podobne komponente negotovosti imajo pri različnih ionih zelo različen učinek na končno nezanesljivost.

Članek objavljen v reviji Talanta (AL26) obravnava primerjavo uporabnosti bližnje IR spektroskopije (NIR) s spektroskopijo v srednjem IR območju, za določanje vsebnosti želatine v papirju. Optimizirali smo referenčno metodo in rezultate uporabili za multivariatno kalibracijo v obeh spektralnih območjih. Referenčna metoda temelji na kromatografskem določanju hidroksiprolina s fluorimetrično detekcijo in je časovno zahtevna. Z uporabo genetskih algoritmov smo optimizirali metodo delnih najmanjših kvadratov in pokazali, da lahko negotovost pri napovedi rezultatov močno zmanjšamo. Srednje IR območje se je izkazalo kot bolj primerno, saj je bila napaka manjša, ker pa je kvalitetna NIR instrumentacija na voljo v prenosni izvedbi, je za analizo vzorcev kulturne dediščine bistveno bolj primerna.

Železo galna črnila, ki imajo izreden zgodovinski pomen, so zaradi vsebnosti kovin korozivna do papirne podlage, s čemer so ogroženi zapisi (AL25). Določanje kislosti (pH) in stopnje depolimerizacije (DP) celuloze v papirju omogoča ugotavljanje stabilnosti in oceno rizika pri rokovanju z zgodovinskimi dokumenti. Z analizo seta vzorcev dokumentov iz 18. in 19. stoletja, smo izdelali metodo osnovano na bližnji infrardeči spektroskopiji (NIR), ki v kombinaciji z metodo delnih najmanjših kvadratov omogoča nedestruktivno določanje pH in DP v zapisih in papirni podlagi. Z izdelano metodo smo analizirali zgodovinske dokumente iz kolekcije Britanskega muzeja in napovedali čas, ko bo zaradi korozije rokovanje z njimi rizično.

Bisfenol A (BPA) je eden glavnih produktov pri termični razgradnji polikarbonata (PC), prav tako pa se izlužuje iz različnih izdelkov narejenih iz PC (AL7). Zaradi visoke akutne toksičnocti BPA, je zmanjševanje nastajanja BPA pri razgradnji PC pomembna problematika. »Infrared Image Furnace« ter »Ion attachment mass spectrometry« tehniki smo uporabili pri raziskavi razvijanja BPA iz PC med segrevanjem le tega bodisi v zraku, bodisi v dušiku. Prav tako smo preizkusili kako vpliva na razgradnjo dodatek $CuCl_2$. Pri termični razgradnji PC precej znižamo nastanek BPA z dodatkom $CuCl_2$, z uporabo dušikove atmosfere ter z uporabo nižjih temperatur segrevanja.

»Ion attachment mass spectrometer« (IAMS) smo uporabili v povezavi z infrardečo pečico (IIF), ki smo jo uporabili za pirolizo vzorcev, za določitev nastalih aromatskih spojin pri pirolizi polietilena (AL13). Učinek dodatka $CuCl_2$ pri pirolizi je bil ovrednoten s primerjavo med razmerjem tvorjenja alkenov in aromatskih spojin med pirolizo. Termogravimetrični eksperimenti in rentgenska praškovna analiza so bili uporabljeni za določitev oksidacijskega stanja bakrovih spojin med potekom pirolize. Redukcija Cu(II) v Cu(I) in nazadnje v Cu(0) je bila okarakterizirana s pomočjo te metode. IIF-IAMS je odlična metoda za »on-line« detekcijo reakcijskih produktov pri eksperimentih s časovno-temperaturno programirano pirolizo.

V delu (AL11) smo v sodelovanju s katedro za anorgansko kemijo študirali nove dvo- in štiri-jedrne komplekse molibdena (V). Pri reakcijah med pirazinom (Pyz = $C_4H_4N_2$) in

$[MoOCl_4(H_2O)]^-$ ali $[MoOBr_4]^-$ so nastali dvojedrni $[(MoOX_4)_2(Pyz)]^{2-}$ (X = Cl, Br), $[\{MoOCl_3(Pyz)\}_2O]^{2-}$ in štirijedrni $[(Mo_2O_4Cl_4)_2(Pyz)_2]^{4-}$ anioni. Vse spojine smo okarakterizirali z rentgensko kristalografijo in IR spektroskopijo. Spojine z $[(MoOX_4)_2(Pyz)]^{2-}$ ioni imajo ireverzibilni elektrokemijski odziv. Temperaturno odvisne magnetne meritve spojin $\{(C_6H_5)_4P\}_2[(MoOX_4)_2(Pyz)]\cdot 2CH_3CN$ kažejo šibke feromagnetne sklopitve preko pirazinskega mostu.

Za potrebe netarčne analize smo izdelali model napovedovanja faktorjev odziva pri GC/MS analizi (AL2). Eksperimentalno smo določili faktorje odziva za masno selektivni detektor za 36 nasičenih in nenasičenih hlapnih organskih spojin, ki vsebujejo ogljikove, vodikove in včasih tudi halogenidne atome. Kemijsko strukturo smo kodirali z različnimi molekularnimi deskriptorji. Za modeliranje smo uporabili multiplo linearno regresijo. Z navzkrižnim validacijskim testom smo določili povprečno napako izračunanih faktorjev odziva na MS detektorju in je bila okoli 15 %, kar zadostuje za določevanje hlapnih organskih snovi v zraku.

V prispevku (AL16) je prikazan vpliv kovinskih ionov na prehodnost fluorokinolonov skozi intestinalne membrane. Na zmanjšano prehodnost fluorokinolonov in s tem njihovo manjšo biodosegljivost lahko vpliva nastanek kompleksov med kovinskimi ioni in fluorokinoloni.

In vivo eksperimenti so pokazali, da kompleksi aluminija s ciprofloksacinom ne prehajajo skozi intestinalne membrane, čemur je lahko vzrok kompleksiranje.

V prispevku (AL10) je prikazan model, ki ponazarja kontinuirno izluževanje nekaterih kovin (B, Cd, Co, Mn, Ni in Sr) iz zemlje v prebavnem traktu. Ekperimentalni podatki, ki so bili pridobljeni z ICP MS, so bili uporabljeni pri izdelavi matematičnega modela. V model sta bila vključena masna prenosa (difuzija iz tekočinskega filma in difuzija s trdne faze) in navidezni difuzijski koeficienti med trdnimi delci. Čeprav so porazdelitveni koeficienti, ki določajo termodinamiko izluževanja posameznih elementov z izjemo B podobni, se profili izluževanja razlikujejo zaradi različnih difuzijskih lastnosti posameznih elementov. Elemente lahko glede na parametre izluževanja razdelimo v več skupin. Rezultati raziskave predstavljajo pomemben prispevek k določevanju protokolov za oceno tveganj.

V zvezi s staranjem in degradacijo papirja in s tem pisne kulturne dediščine, je bil izdelan in patentiran postopek in metoda za kemijsko stabilizacijo papirja. Patent (AL49) se nanaša na sintezo antioksidanta in metodo za njegovo aplikacijo za zaščito pisnih gradiv na papirju. Antioksidant ima lastnost preprečevanja, upočasnitve ali poprave poškodb zaradi oksidacije in/ali kislinske hidrolize in ne kaže slabosti prej uporabljenih formulacij.

b)

Hlapni aldehidi nastajajo pri razgradnji papirnatih materialov. To je lahko vzrok za njihovo akumulacijo v arhivskih in knjižničnih skladiščih. Kljub temu do sedaj še ni bilo opravljene sistematične študije. V okviru raziskave (AL5) je bilo izvedeno pasivno vzorčevanje na desetih lokacijah v štirih arhivih in knjižnicah. Kljub zelo različnim vzorčevalnim lokacijam, ni bilo večjih razlik. Lahko pa rečemo, da so v zračenih skladiščih najnižje koncentracije hlapnih aldehidov, medtem ko so v nezračenem skladišču časopisov koncentracije hlapnih aldehidov najvišje (formaldehid, acetaldehid, furfural in heksanal). Preverili smo tudi izpostavljenost osebja hlapnim aldehidom, tako da je pet oseb iz ene inštitucije uporabilo pasivne osebne vzorčevalnike. Vse vsebnosti so bile nižje od trenutno predpisanih za izpostavljenost delavcev.

Koncentracije hlapnih aldehidov, ocetne kisline in celokupnih hlapnih organskih spojin (HOS) smo primerjali s koncentracijami onesnaževal v zunanji atmosferi. Opazili smo, da je v skladiščih, še posebno v arhivskih škatlah, koncentracija HOS in ocetne kisline precej večja kot

koncentracija onesnaževal iz zunanje atmosfere, ki se rutinsko spremljajo v povezavi z materiali kulturne dediščine. To je razlog, da so potrebne nadaljne raziskave na področju učinka razgradnje HOS na materiale kulturne dediščine in da je potrebno uvesti spremljanje vsebnosti HOS v kulturnih inštitucijah.

V delu (AL8), predlagamo novo testno metodo za vrednotenje primernosti konzervatorskih materialov in materialov za hrambo objektov kulturne dediščine. Test se izvaja 5 dni na temperaturi 100 °C v zaprtih vialah, v katerih sta testni material in referenčni papir. Hlapne spojine, ki izhajajo iz referenčnega materiala lahko povzročijo razgradnjo referenčnega papirja in posledično zmanjšajo njegovo stopnjo polimerizacije. Le to določamo z uporabo viskozimetrije. Predlagamo optimalno vrsto vial, ki zagotavlja ponovljivost rezultatov s standardno deviacijo eksperimentov s tremi paralelkami pod 2 %. Izbran referenčni material, filter papir Whatman št. 1, narejen iz očiščenih bombažnih vlaken, je občutljiv na hlapne spojine, ki pospešujejo razgradnjo s hidrolizo in oksidacijo. Posledično lahko predvidimo vpliv testiranega materiala na razgradnjo organskih materialov in objektov kulturne dediščine. Ta raziskava opiše več načinov uporabe predlagane metode in predstavi izrazit vpliv lesovinskega papirja na razgradnjo referenčnega papirja. Preiskovali smo tudi različne kombinacije z ročnim, lesovinskim in recikliranim papirjem, prav tako pa smo evalvirali večje število kartonov, ki se uporabljajo za shranjevalne ovitke in škatle. Predlagan, nov test je ponovljiva, poceni in hitra metoda za ugotavljanje ustreznosti materialov za shranjevalna oziroma razstavna ohišja, v katerih so objekti kulturne dediščine organskega izvora. Na ta način bi omogočili konzervatorjem, izdelovalcem konzervatorskih materialov in upravljalcem zbirk boljšo izbiro materialov za ohišja namenjena shranjevanju in razstavljanju eksponatov.

Železo galna črnila imajo visoko vsebnost kislin in prehodnih kovin, zato pospešujejo razgradnjo celuloze s hidrolizo in oksidacijo (AL22). Njihova kemijska interakcija z okoljem ni dobro raziskana, še posebej s stališča emisij razgradnih produktov, ki lahko vplivajo na intenzivnost razgradnih procesov. Pri študiju emisij smo uporabili mikroekstracijo na trdno fazo v povezavi s plinsko kromatografijo in masno spektrometrijo. Za identifikacijo in kvantifikacijo hidroksilnih radikalov smo uporabili tekočinsko kromatografijo. Prav tako smo študirali kemiluminescenco celuloze, ki je bila razgrajena zaradi črnila. Pokazali smo, da so emisije hlapnih organskih razgradnih produktov kot posledica vpliva črnila manj intenzivne kot emisije iz okoliškega papirja, čeprav črnilo pospešuje razgradnjo celuloze tudi na večjih razdaljah (z objekta na objekt). To smo povezali z emisijami reaktivnih kisikovih spojin, najverjetneje z vodikovim peroksidom, saj so emisije le tega bolj intenzivne iz črnila kot iz okoliškega papirja.

Raziskovali smo obstojnost organskih barvil (lakov) med razgradnjo pod vplivom svetlobe (AL23). Pri raziskavah smo uporabili kemiluminometrijo, viskozimetrijo in kolorimetrijo. Razvili smo metodo, pri kateri smo vzorec obsevali s sprednje strani, kemiluminescentni signal pa smo merili s hrbtne strani vzorca. Kompleksno razmerje med sestavo papirja in sestavo barvila ter vplivi na razgradnjo smo raziskali z uporabo multivariantne analize. Ugotovili smo, da imajo kromofori pro-oksidativno vlogo, pri čemer imajo vpliv tudi prehodne kovine.

Znano je, da so barvila v barvnih fotografijah občutljiva na pogoje hrambe, kljub temu pa ni podatkov o njihovi obstojnosti v onesnaženi atmosferi (AL23). Zato smo stabilnost primerjali pri pogojih pospešene razgradnje pri povišani temperaturi, s tem da smo preverili vpliv formaldehida, ocetne kisline in dušikovega dioksida. Obstojnost smo izrazili relativno z uporabo kolorimetrične metode, pravilnost rezultatov slednje pa smo preverili z ekstrakcijo barvil in tekočinsko kromatografijo. Ugotovili smo, da na obstojnost najbolj vpliva prisotnost ocetne kisline, ki je hkrati tudi prisotna v največji koncentraciji v arhivski atmosferi. Po drugi strani se je izkazalo, da ima formaldehid celo nekoliko pozitiven učinek na obstojnost.

Razvili smo metodo za elektrolitsko nanašanje zlitin Fe–Pd, ki imajo po termični obdelavi odlične magnetne lastnosti (AL14). Kot katoda je služila plast Au nanešena na steklo, s pravilno kombinacijo elektrolita, ligandov in napetosti pa smo kontrolirali vsebnost posamezne kovine v zlitini. Plasti Fe–Pd so bile debele okrog 200 nm, po elektrolizi pa smo jih obdelali termično med 400 in 600 ºC za 1 h v zmesi Ar, ki je vseboval 7 % H_2. Pokazalo se je, da ima temperatura pomembno vlogo pri intergranularni difuziji sestavin, optimalno koercitivnost 870 Oe pa smo dosegli pri 400 ºC.

c)

V članku objavljenem v reviji Food Chemistry (AL12), obravnavamo primerjavo izolacijskih metod pri določanju hlapnih spojin v ajdi. Pri določanju spojin arome ajde smo kombinirali pet različnih izolacijskih tehnik s plinsko kromatografijo – masno spektrometrijo: dinamična »headspace« tehnika (DHS) s hladno pastjo ali pastjo s sorbentom, mikroekstrakcija na trdno fazo (SPME), ekstrakcija na mešalo s sorbentom (HSSE), ekstrakcija s topili (SE) in destilacija s hkratno ekstrakcijo (SDE). Predstavljamo način optimizacije vsake tehnike ter primerjavo kemijskih profilov spojin, ki smo jih z njimi izolirali. Pri ekstrakciji s topilom metanolom smo izolirali dokaj polarne in manj hlapne spojine ter smo jo označili kot najmanj primerno za določitev spojin, odgovornih za vonj. Samo SPME z vlaknom DVB/CAR/PDMS je bila primerna za izolacijo zelo hlapnih spojin v širokem območju polarnosti. Z DHS se je ekstrahiralo najmanj spojin, vendar je bil kemijski profil podoben kot pri SDE, ki smo jo tudi izbrali kot najbolj primerno tehniko za določitev spojin arome kuhane ajde. Uporabljene izolacijske tehnike se dopolnjujejo glede možnosti ekstrakcije reprezentativnega profila arome ajde.

Ajda je žito z močno karakteristično aromo. Pred kratkim smo identificirali spojine (AL6), odgovorne za aromo ajdovega zdroba, vendar pa še ni poznana njihova porazdelitev med različne dele ajdovega zrnja (moka, otrobi, luščine). V tej študiji smo raziskovali sestavo spojin arome v posameznih delih ajdovega zrnja ter jo primerjali s sestavo spojin arome v zdrobu, pridobljenem iz istega ajdovega zrnja. Hlapne spojine iz vsakega vzorca smo ekstrahirali z destilacijo s hkratno ekstrakcijo (SDE) z Likens-Nickersonovim aparatom. Ekstrakte smo analizirali s plinsko kromatografijo v povezavi z masno spektrometrijo (GC-MS) z elektronsko ionizacijo. Poleg spojin arome, ki so bile prisotne v vseh frakcijah, so bile nekatere spojine prisotne le v moki in otrobih, ne pa v zdrobu. Nadalje smo nekatere spojine identificirali samo v ajdovem zdrobu, ne pa v moki ali otrobih: oktanal, *E,E*-2,4-heptadienal, *E*-2-decenal, *E,E*-2,4-dekadienal. Spet druge smo identificirali le v luščinah: *E*-2-heksenal, heptanal, *E,E*-2,4-heksadienal, fenilacetaldehid in α-bisabolol.

Raziskovali smo vpliv pH, vrste topila in UV svetlobe na stabilnost statinov (AL9). Rezultati kažejo močan vpliv pH in UV žarkov na degradacijo, ki poteka preko vzbujenega singletnega stanja pri vzbujanju v π–π^* pas. Degradacija statinov v vodi je precej nižja, kot če uporabimo kot topilo acetonitril.

Študirali smo stabilnost enalaprilijevega maleata (AL15). Ta učinkovina se uporablja za regulacijo krvnega tlaka. Za študij stabilnosti smo razvili analizne metode, ki omogočajo ločevanje zelo podobnih razpadnih produktov in njihovo identifikacijo. Z uporabo visokoločljivostnega masnospektrometričnega detektorja v MS^n varianti po ločevanju nečistoč z UPLC, smo nastale nečistote tudi identificirali.

V prispevku (AL1) je opisan postopek za določevanje Ni v farmacevtskih preparatih z elektrotermično atomsko absorpcijsko spektrometrijo. Opisan je postopek priprave z mikrovalovnim razkrojem ter optimiranje eksperimentalnih pogojev merjenja. Natančnost postopka je zado-

voljiva (r.sd pod 4 %), meja kvantifikacije pa 2 μg/g. Postopek je primeren za določevanje sledov Ni v različnih farmacevtskih preparatih in surovinah.

Opisan je postopek za določevanje Cd, As in Pb v rečnih sedimentih (AL18). Priprava vzorcev je temeljila na mikrovalovnem razkroju z uporabo dušikove (V), klorovodikove in fluorovodikove kisline ter dodatku borove kisline za kompleksiranje fluoridnega iona. Uporabljeni so bili različni matrični modifikatorji, med katerimi je bila pri določevanju Cd in Pb najprimernejša dušikova (V) kislina, pri določevanju As pa mešanica paladijevega im magnezijevega nitrata. Pravilnost postopka je bila preverjena s certificiranimi referenčnimi vzorci. Določena je bila natančnost postopka, meje zaznave in meje določljivosti. Metoda je bila uporabljena za analizo realnih vzorcev.

V članku (AL18) smo opisali klasifikacijo mediteranskih merilnih postaj za merjenje fotokemijskih onesnaževal. Nedavno vpeljane fotokemijske indikatorje P1 in P2 smo uporabili za klasifikacijo onesnaženosti merilnih postaj za določevanje koncentracij troposferskega ozona, ki so locirane v Mediteranskih pokrajinah Hrvaške, Italije in Slovenije. Omenjeni indikatorji nam prav tako omogočajo spremljanje letnih trendov fotokemijske produkcije ozona v omenjenem območju. Najboljši klasifikator se je izkazal kvadratni koren njunega produkta.

Epifitski lišaj (*Hypogymnia physodes)* je bil uporabljen pri študiju onesnaženja zraka na področju mesta Sarajeva (AL19). V lišajih, odvzetih s petih lokacij mesta Sarajeva, je bilo z ICP-MS določenih 14 elementov. Rezultati kažejo znatna povišanja koncentracij Cr, Pb in Zn, glede na primerjalne vrednosti v vzorcih, odvzetih na področjih severozahodne Evrope.

Nadaljevali smo s karakterizacijo produktov v utekočinjenem lesu (AL20). V destilatu po utekočinjenju smo določili predvsem furfural v konc. okoli 500ppm. Študirali smo tudi uporabnost nekaterih lesnih gljiv za razgradnjo endosulfana. Ugotovili smo, da predvsem glive *H. fragiforme* v tekoči kulturi dobro razgrajujejo endosulfan.

Delo (AL21) obravnava možnosti mikoremediacije lindana v tekočih kulturah gliv *Pleurotus ostreatus* in *Hypoxlon fragiforme.*

Zaščitni pripravki na osnovi borovih spojin sodijo v skupino najpomembnejših biocidov za zaščito lesa (AL27). Zmanjšanje izpiranja in s tem večjo učinkovitost borove kisline smo poskušali doseči tako, da smo ji dodali vodno emulzijo voska montana. Vzorce smrekovega lesa smo impregnirali in izpirali po novih postopkih OECD in prCEN/TS 15119-1. Dodatek emulzije ne vpliva bistveno na izpiranje borove kisline. Pokazalo pa se je, da je postopek OECD mnogo rigoroznejši kot prCEN/TS 15119-1.

Biocidi na osnovi bora sodijo med učinkovite fungicide in insekticide (AL29). Ker pa se na les ne vežejo, so močno podvrženi izpiranju. Da bi izpiranje zmanjšali, smo pripravili polietilensko emulzijo (WE1) in oksidirano polietilensko voskano emulzijo (WE6) v kombinaciji z borovo kislino. Vzorce smrekovega lesa smo vakuumsko impregnirali in nato izpirali v skladu s procedurami, opisanimi v prCEN/TS 15119-1, ENV 1250-2 in EN 84. Rezultati so pokazali, da se večina borove kisline izpere že v prvem ciklusu izpiranja. WE6 emulzija v kombinaciji s termično obdelavo izpiranje do neke mere zmanjša.

Programska skupina je sestavljena iz sodelavcev zaposlenih na FKKT UL kjer večino delovnega časa namenimo izobraževanju in usposabljanju strokovno izobraženih kadrov na področju kemije in njenih specializiranih znanstvenih disciplin. Poleg prenašanja znanj na dodiplomske in podiplomske študente, so bili sodelavci PS v letu 2010 mentorji 26 diplomantom ter mentorji oz. somentorji trem magistrandom in sedmim doktorandom, ter na ta način pomembno

prispevali k usposabljanju kadrov, neobhodno pomembnih za kemijsko industrijsko proizvodnjo ter različne raziskovalne inštitucije.

RESEARCH PROGRAMME REPORT

RESEARCH TOPICS AND GOALS

a) Basic research in analytical methods and approaches
b) Research and development of methods for the analysis and characterisation of materials
c) Development of methods and procedures for quality control in industrial production, food safety and environment.

SCIENTIFIC AND OTHER RELEVANT ACHIEVEMENTS

During 2010, members of the programme group published 30 original scientific articles (AL1–AL30) and two short communication articles (AL31-AL32), delivered one invited lecture (AL33), eleven lectures on scientific conferences (AL34-AL44) and acquired one European patent (AL49).

The following subjects were studied:

a)

Novel method for fast characterization of high-surface-area electrocatalytic materials using a carbon fiber microelectrode was developed (AL17**)**. A carbon fibre microelectrode (CFME) was used for characterization of the nanoparticle catalysts as an alternative to the well-established rotating disk electrode (RDE) method. We found out that the novel CFME method yielded comparable results to the RDE method when investigating the adsorption/desorption processes as well the specific activity for reactions such as the oxygen reduction reaction. Its major advantage over the RDE method is a fast sample preparation and rapid measurement, reducing significantly the time of a single sample characterization from 2–3 h to a favourable 5–10 min.

Prussian blue (PB) modified titanate nanotubes (PB-TiNT) have been synthesized by the reaction of Fe^{2+}-modified TiNT with hexacyanoferrate(III) ions (AL28). The rate constant for heterogeneous catalytic reaction between PB-TiNT and H_2O_2 was found to be $k = 2.10^4$ $dm^{3/}$ (mol s), which is an order of magnitude higher than the values of *k* reported for conventionally prepared, electrochemically deposited PB films. On the PB-TiNT modified electrode with subnanomolar surface concentration of PB (Γ(PB) = $2.8.10^{11}$ mol/cm^2), a stable, reproducible and linear response towards H_2O_2 was obtained in the concentration range 0.02–4 mM, with the sensitivity of 0.10 $AM^{-1}cm^{-2}$ at –150 mV.

A general methodology for a systematic evaluation of the uncertainty was derived (AL3**)** for each particular ion in stock combined calibration standards in which concentrations of different ions extend over up to five orders of magnitude resulting in detailed uncertainty budgets with the aim of recognising the major contributions to combined uncertainties. This work confirmed that it is justifiable that the mass fraction of impurities in other chemicals is taken into account when calculating the mass concentration of an ion in combined calibration standard solution similarly to what is already common practice in accounting for the purity of chemical.

It was proven that impurities in chemicals, which are the sources of major ions, have significant effect on uncertainty budget of minor ions; already if the major ion exceeds 25 times the minor ion's concentration. For several ions it was confirmed that mass fraction of the impurities was the major source of uncertainty

Article (AL4) deals with the development and application of the detailed uncertainty budget for simultaneous determination of minor and major ions in seawater and derived saline solutions. Combination and sequence of gravimetric or/and volumetric steps involved in introducing each particular ion into stock and final combined calibration standards; cross contamination of chemicals and dilution of samples were critically assessed and their significance to the combined uncertainty was evaluated. The main uncertainty components were identified and quantified for all anions and cations determined with ion chromatography in seawater and estuary water and confronted with uncertainties associated with concentrations of ions in combined calibration standards. Similar uncertainty components reflect very differently upon different ions.

Quantitative non-destructive analysis of individual constituents of historic rag paper is crucial for its effective preservation. In the work published in Talanta (AL26), we examine the potentials of mid- and near-infrared spectroscopy. In order to fully utilise the selectivity inherent to spectroscopic multivariate measurements, genetic algorithms were used to select spectral data derived from information-rich FT-IR or UV-vis-NIR measurements to build multivariate calibration models based on partial least squares regression, relating spectra to gelatine content in paper. A selective but laborious chromatographic method for the quantification of hydroxyproline (HYP) has been developed to provide the reference data on gelatine content. We used 9-fluorenylmethyl chloroformate (FMOC) to derivatise HYP, which was subsequently determined using reverse-phase liquid chromatographic separation and fluorimetric detection. In this process, the sample is consumed, which is why the method can only be used as a reference method. The sampling flexibility afforded by small-size field-portable spectroscopic instrumentation combined with chemometric data analysis, represents an attractive addition to existing analytical techniques for cultural heritage materials.

Considering that iron gall inks have been used for over a millennium they have extraordinary historical significance (AL25). Due to their corrosiveness, which is a consequence of their acidity and content of transition metals, iron gall inks accelerate the degradation of old scriptures or drawing support, in this study rag paper. Characterisation of the acidity (pH) and degree of polymerisation (DP) of cellulose in paper is thus of high relevance as it enables the estimation of material stability and assessment of risks associated with its handling. Based on a well-characterised set of samples with iron gall ink from the 18th and 19th centuries, we developed a near infrared spectroscopic method with partial least squares calibration for non-destructive determination of pH and DP of both inked areas and paper. Using this method, we analysed 27 iron gall ink drawings from the 18th and 19th century from the British Museum collection. In all cases, inked areas turned out to be more acidic and degraded more rapidly than the surrounding paper. Based on the DP data obtained, we were able to estimate the degradation time needed for the inked areas to the point when they could become at risk of damage due to handling. Using the average uncertainty of the calculated lifetime, we proposed a quantitative stability classification method which could contribute to the curatorial and conservation decision-making process.

Bisphenol A (BPA), which is a well-known endocrine disruptor (AL7), is one of the major products in thermal degradation of polycarbonate (PC) and is also leached out from various PC products. Because of high acute toxicity of BPA, reducing BPA production during degradation

of PC is an important topic. A combined Infrared Image Furnace with Ion attachment mass spectrometry technique was used to investigate the evolution of BPA from a PC sample during heating in either nitrogen or air atmosphere, and with or without a $CuCl_2$ catalyst. Thermal treatment in the presence of $CuCl_2$, in nitrogen atmospheres and at lower degradation temperatures, substantially reduced the BPA emission.

Infrared image furnace ion-attachment mass spectrometry (IIF-IAMS) experiments have been conducted to elucidate the effects of copper(II) chloride on the formation of aromatic compounds during the pyrolysis of polyethylene (AL13). Under the time-resolved pyrolysis conditions of IIF-IAMS, the effects of $CuCl_2$ were measured to compare the variation in ratios of alkenes and aromatics during polyethylene thermal degradation when pyrolysis temperature was increased. Thermogravimetry experiments and X-ray powder diffraction analysis conducted under similar conditions to those used for IIF-IAMS allowed for characterisation the oxidation states of copper prevailing during the thermal degradation process of polyethylene in the presence of $CuCl_2$. Reduction of Cu(II) into Cu(I) during the pyrolysis process was characterized. The IIFIAMS method demonstrated its advantage for on-line detection of reaction products during the time-resolved pyrolysis experiments.

Reactions of pyrazine (Pyz = $C_4H_4N_2$) with $[MoOCl_4(H_2O)]^-$ or $[MoOBr_4]^-$ afforded a series of complexes, dinuclear $[(MoOX_4)_2(Pyz)]^{2-}$ (X = Cl, Br), $[\{MoOCl_3(Pyz)\}_2O]^{2-}$ and tetranuclear $[(Mo_2O_4Cl_4)_2(Pyz)_2]^{4-}$ anions, with N-donor ligands engaged either in monodentate or bidentate bridging coordination (AL11). A dinuclear $[(MoOX_4)_2(Pyz)]^{2-}$ ion, which may be viewed as a linkage of two mononuclear subunits with a bidentate pyrazine, crystallizes either as a PyH^+ (pyridinium cation, $C_5H_5NH^+$; compound **1**), a $\{(C_2H_5)_4N\}^+$ (compound **2**) or a $\{(C_6H_5)_4P\}^+$ salt (compounds **3** and **4**). In $(PyH)_2[\{MoOCl_3(Pyz)\}_2O]$ (**5**) with an *anti*-$\{Mo_2O_3\}^{4+}$ core, pyrazine is bound to the metal through only one nitrogen atom. The tetranuclear $[(Mo_2O_4Cl_4)_2(Pyz)_2]^{4-}$ ion, a linkage of two metal–metal bonded $\{Mo_2O_4\}^{2+}$ cores with a pair of bidentate pyrazines, is found in two compounds, $(MeNC_5H_5)_2(PyzH_2)$-$[(Mo_2O_4Cl_4)_2(Pyz)_2]$ (**6**) [$MeNC_5H_5^+$ = *N*-methylpyridinium cation, $PyzH_2^{2+}$ = pyrazinium(2+) cation] and $(PyH)_4[(Mo_2O_4Cl_4)_2(Pyz)_2]\cdot 2CH_3CN$ (**7**). In the presence of methanol, dinuclear $\{(C_6H_5)_4P\}_2[(MoOBr_4)_2(Pyz)]\cdot 2CH_3CN$ (**4**) was transformed directly into tetranuclear $(PyH)_4[(Mo_2O_4Br_4)_2(Pyz)_2]\cdot 2CH_3CN$ (**8**). All compounds were fully characterized by X-ray crystallography and IR spectroscopy. The compounds containing the $[(MoOX_4)_2(Pyz)]^{2-}$ ions display an irreversible electrochemical reduction behaviour. Temperature-dependent magnetic measurements on $\{(C_6H_5)_4P\}_2[(MoOX_4)_2(Pyz)]\cdot 2CH_3CN$ (X = Cl for **3**, X = Br for **4**) reveal a weak ferromagnetic coupling across the pyrazine bridge between a pair of MoV $S = 1/2$ spins. The magnetic properties of $\{(C_2H_5)_4N\}_2[(MoOCl_4)_2(Pyz)]$ (**2)** are dominated by antiferromagnetic intermolecular interactions.

Experimental MS response factors were measured for 36 different saturated and unsaturated volatile organic compounds (VOC), containing carbon, hydrogen and halogen atoms (AL2). Chemical structure was encoded using various molecular descriptors. A quantitative structure-property relationship model was established using multiple linear regression models. The cross-validation ability of the created model was estimated by leave-one-out cross-validation procedure. Error in the cross-validation of response factors was calculated by cross-validation procedure and was 15%, which is sufficient for the determination of VOCs in the air. The proposed procedure can be used for simultaneous qualitative and quantitative determination of volatile organic compounds in the atmosphere.

Interactions between a fluoroquinolone antimicrobial agent and metal cations were studied (AL16) on rat intestine membrane in vitro to prove if the decreased quinolone intestinal per-

meability is caused by complex formation between metal cations and fluoroquinolones. We found that the fluoroquinolone permeability decreased in the presence of metal cations and the obtained results show that the ciprofloxacin–aluminum complex does not permeate the intestinal mucosal membrane.

Physical processes which control the desorption of some elements (B, Cd, Co, Mn, Ni, and Sr) from soils in a continuous leaching system representing the human stomach were investigated (AL10) by fitting experimental leaching data to a mathematical particle diffusion model. Soil samples (50 mg) from Cornwall, UK, contained in a flowthrough extraction chamber (ca. 6.5 mL) were intimately contacted with artificial gastric solution at various flow rates (0.42–1.42 mL min-1) for up to ca. 4 h, followed by the analysis of fractions collected with inductively coupledplasma massspectrometry (ICPMS). The leaching profiles of the various elements were fitted to a mathematical model incorporating two mass transfer processes (liquid film diffusion and apparent solid phase diffusion) to determine the effective external mass transfer coefficient (β) and the apparent intraparticle soil diffusion coefficient (D_a). A system of partial differential equations was solved numerically with finite difference discretization of the computational domain allowing the rate limiting physical desorption process(es) for each element to be determined. The (thermodynamic) driving force of the leaching process was defined by the distribution coefficient(Kd0) between soil and leachant.

Although the K_{d0} values investigated were very similar (ca. 6–15L kg-1) for the elements studied with the exception of B (ca. 2.7 Lkg-1), the leaching profiles were much different due to diffusion limited processes. The elements may be classified as limited by β (B, Sr, and Cd), by D_a (Co, and Mn) or by β and D_a (Ni). This results in quantifiable parameters for the liability of elements in soil upon ingestion, which may be implemented in future risk assessment protocols.

The object of the invention (AL49) was to provide alternative antioxidants for treating organic material, particulary paper, which can prevent, slow down or reverse damage due to oxidation reactions and/or acid hydrolysis reactions and do not exhibit the disadvantages of previously used formulations.

b)

During degradation of paper-based materials volatile aldehydes are produced which may be accumulating in archival and library repositories. However, no systematic study has been performed so far. Within the framework of this study (AL5), passive sampling was carried out at ten locations in four libraries and archives. Despite very different sampling locations, no major differences were found. However, in airfiltered repositories lower concentrations were found, while non-ventilated newspaper repositories exhibited highest concentrations of volatile aldehydes (formaldehyde, acetaldehyde, furfural and hexanal). Five employees in one institution were also provided with personal passive samplers to investigate employees' exposure to volatile aldehydes. All values proved to be lower than the presently valid exposure limits.

The concentrations of volatile aldehydes, acetic acid, and volatile organic compounds (VOCs) in general were also compared with those of outdoor-generated pollutants. It was evident that inside the repository, and particularly inside archival boxes, the concentrations of VOCs and acetic acid were much higher than the concentration of outdoor-generated pollutants, which are otherwise more routinely studied in connection with heritage materials. This indicates that further work on the pro-degradative effect of VOCs on heritage materials is necessary and that monitoring of VOCs in heritage institutions should become more widespread.

To evaluate the compatibility of conservation and storage materials with heritage objects of organic origin, a new test method is proposed (AL8). The test was performed in closed vials at 100 °C for 5 days with the tested material and a reference paper in the vial. Volatiles off-gassed from the tested material may cause degradation of the reference paper and lead to a decrease in its degree of polymerization. This was determined by using viscometry. The optimal vial type is proposed, leading to reproducible results with a standard deviation for three parallel experiments typically under 2%. The selected reference material, Whatman No. 1 filter paper, made of purified cotton linters, is susceptible to volatiles and promotes both, hydrolytic and oxidative degradation, and its response to tested materials is thus likely to be relevant to a wide variety of heritage materials and objects of organic origin. The case studies show possible applications of the proposed method, and a pronounced pro-degrading effect of groundwood containing paper on the reference paper is shown, a variety of combinations of rag, groundwood and recycled papers were studied and a number of cardboards used for wrapping or for boxes were evaluated. The new test is proposed as a repeatable, inexpensive and rapid method of assessment of compatibility of materials used for housing or display of heritage objects of organic origin, thus enabling conservators, providers of conservation materials and collection managers to make better informed selection of appropriate housing or display materials.

Iron gall inks are characterised by high contents of acids and transition metals, promoting degradation of cellulose due to hydrolysis and oxidation, respectively (AL22). Their chemical interaction with the environment is not well understood, especially in view of emissions of degradation products which could lead to spreading the degradation processes. In order to study the emissions, we employed gas chromatography/mass spectrometry following headspace micro-extraction, and liquid chromatography following hydroxyl radical scavenging with appropriate probes. We also studied chemiluminescence of cellulose affected by ink degradation. We show that while the emissions of organic volatile degradation compounds by inks are less intense than those of surrounding paper, ink promotes the degradation of cellulose across big distances (from object to object). We were able to link this to emission of reactive oxygen species, probably hydrogen peroxide. Its emission from ink is considerably more intensive than from paper.

The photo degradation of watercolour drawings prepared with madder lake pigments on gelatine-sized paper was studied by chemiluminometry, viscometry, and colorimetry (AL23). A method of recto irradiation and verso measurement was developed to overcome absorption of the emitted photons by the paint layer. A complex relationship between paper substrate, applied chromophores and associated transition metals was observed with strong correlations between the presence of transition metals associated with the madder lakes and the degradation of the paper substrate and the applied paint layer, as well as evidence of pro-oxidative activity by the chromophores in the applied paint layers. The pro-oxidant behaviour appears to be dependent on the type of transition metal present. This is the first in-depth research into the photodegradation of madder lake-based watercolours which attempts to understand the chemistry of the processes.

Chromogenic colour prints are known to be sensitive to storage environments (AL23). However, limited research is available on the effect of atmospheric pollutants on these materials, especially indoor pollutants. The stability of photographic dyes is of particular interest and the rate of their change can be best described using the standard RGB colour model. Therefore, the colourimetric method was compared to dye extraction and liquid chromatographic analysis to justify its use as a rapid, non-destructive method for quantitative assessment of the rate of change in dye content of colour photographs during degradation. The effects of typical indoor (acetic acid, formaldehyde) and outdoor (nitrogen dioxide) generated pollutants on chromog-

enic colour prints were then investigated at 80 °C, 60% RH. It was identified that acetic acid leads to the most pronounced changes in photographic dye concentrations. This is significant, considering that acetic acid is often the most prominent pollutant in archival environments. On the other hand, formaldehyde exhibited a slight protective effect in comparison to the blank experiment.

Equiatomic Fe–Pd thin films with thicknesses of 200 nm were deposited from a single electrolyte onto glass-based, Au-coated substrates using the electrodeposition method (AL14). Such deposited films were annealed at temperatures from 400 to 600 °C for 1 h in Ar+7% H_2. The phase formation, microstructure and the magnetic properties were analyzed. The $L1_0$ ordering was found to coincide with the grain growth and the interdiffusion reaction between the substrate and the thin film when temperatures above 500 °C were used, which resulted in lower coercivities. The highest coercivity of 870 Oe was achieved when modest temperatures (400 °C) were used.

c)

Five different isolation techniques were combined with gas chromatographic–mass spectrometric determination of aroma compounds from buckwheat (AL12): dynamic headspace (DHS) with cryotrapping or sorbent trapping, solid-phase microextraction (SPME), headspace sorptive extraction (HSSE), solvent extraction (SE) and simultaneous distillation–extraction (SDE). Optimisation of each technique is presented, as well as comparison of the chemical profiles obtained by them. Solvent extraction with methanol resulted in the isolation of rather polar and less volatile compounds and was deemed least suitable for the odour-active compounds. Only SPME with DVB/CAR/PDMS fibre was suitable for the isolation of highly volatile compounds in a wider polarity range. DHS extracted the smallest number of compounds, however with comparable chemical profile as obtained by SDE, which was chosen as the most suitable technique to obtain the aroma compounds of cooked buckwheat. The applied isolation techniques are complementary in their ability to extract a representative aroma profile of buckwheat.

Buckwheat is a pseudocereal with a strong characteristic aroma. Compounds responsible for the aroma of buckwheat groats were recently identified (AL6), but the distribution of aromatic compounds between different fractions of the buckwheat kernel (flour, bran, and husk) is not yet known. In this study, the composition of aromatic compounds in buckwheat seed fractions was investigated and compared to the composition of aromatic compounds in groats produced from the same batch of buckwheat seeds. Volatiles from each sample were extracted with simultaneous distillation/extraction with a Likens-Nickerson apparatus. Extracts were analyzed by gas chromatography coupled with mass spectrometry (GC-MS) with electron ionization. Apart from the aroma molecules present in all fractions, compounds which are present only in flour or bran, but not in groats, were also found. Furthermore, some compounds were identified only in buckwheat groats but not in buckwheat flour or bran [octanal, (*E*,*E*)-2,4-heptadienal, (*E*)-2-decenal, and (*E*,*E*)-2,4-decadienal], others were identified only in husks [(*E*)-2-hexenal, heptanal, (*E*,*E*)-2,4-hexadienal, phenylacetaldehyde, and alpha-bisabolol].

In study (AL9) we investigated the stability of statin drugs in different conditions, such as various pH, diverse solvents ratio, presence of UV, and sunlight. The results suggest strong dependence of statins upon pH, potential environmental persistence towards sun light, and UV light degradation via singlet excited state obtained by excitation into the π–π^* band. In acidic conditions, interconversion is retarded between lactone and hydroxy acid forms in aqueous solutions at room temperature, while it is accelerated the same sun-exposed samples. Longer exposures lead to the degradation processes. Statin interconversion in water is much

lower than in acetonitrile. In the article (AL15) we investigated the stability of enalaprilium maleate.

We developed an electrothermal atomic absorption spectrometric procedure for the determination of nickel in active pharmaceutical ingredients (AL1). Since the recoveries of nickel by direct dissolution of samples in diluted nitric acid were low and caused errors in the determination of Ni in pharmaceutical samples, different approaches for sample pretreatment were examined. It was found that the microwave digestion was the most suitable way for sample preparation. Various combinations of digestion agents and different microwave conditions were tested. The most appropriate combination was found to be nitric acid and hydrogen peroxide. The validity of the method was evaluated by recovery studies of spiked samples and by the comparison of the results obtained by inductively coupled plasma mass spectrometry (ICP-MS). The recovery ranged from 87.5 to 104.0% and a good agreement was achieved between both methods. The detection limit and the limit of quantification were 0.6 and 2.1 μg g–1 respectively. The precision of the method was confirmed by determining Ni in the spiked samples which was below 4%, expressed in terms of a relative standard deviation. The method was applied to the determination of nickel in production samples of active pharmaceutical ingredients and intermediates.

The applicability of nitric acid, palladium nitrate and a mixture of palladium and magnesium nitrate as matrix modifiers (AL18) was estimated for accurate and reproducible determination of cadmium (Cd), lead (Pb) and arsenic (As) in sediments of the Sava river by electrothermal atomic absorption spectrometry, ETAAS. Decomposition of the samples was done in a closed vessel microwave-assisted digestion system using nitric, hydrochloric and hydrofluoric acids, followed by the addition of boric acid to convert the fluorides into soluble complexes. The parameters for the determination of Cd, Pb and As in sediments were optimised for each individual element and for each matrix modifier. In addition, two sediment reference materials were also analysed. In determination of Cd and Pb, nitric acid was found to be the most appropriate matrix modifier. The accurate and reliable determination of Cd and Pb in sediments was possible also in the presence of boric acid. The use of a mixture of palladium and magnesium nitrate efficiently compensated for matrix effects and allowed for accurate and reliable determination of As in the sediments. Quantification of Cd and As was performed by calibration using acid matched standard solutions, while the standard addition method was applied for the quantification of Pb. The repeatability of the analytical procedure for the determination of Cd, Pb and As in sediments was ±5% for Cd, ±4% for Pb and ±2% for As. The *LOD* values of the analytical procedure were found to be 0.05 mg/kg for Cd and 0.25 mg/kg for Pb and As, while the *LOQ* values were 0.16 mg/kg for Cd and 0.83 mg/kg for Pb and As. Finally, Cd, Pb and As were successfully determined in sediments of the Sava river in Slovenia.

Ozone data from 19 Italian, Slovenian and Croatian monitoring stations for the period from 2000 and onwards (AL18) were used to calculate the recently introduced photochemical indicators P1 and P2 during the growth season from 1 April to 30 September (Kovac-Andric et al., 2009). The highest indicator values were found in stations from the lower Po river valley and along the northern Italian Adriatic coast. The data collected from 4–5 years show that the average yearly ozone volume fraction in the region remains constant or slightly decreases despite substantial year-to-year fluctuations. An exception was observed in year 2003 when a strong increase of ozone production of up to 25 was observed, with an exception of three southern Italian sites (Sacco, Fontechiari and Ce54) and then a significant decrease ocurred in 2004 (however at the three sites above a slight increase was found instead). In cases when P1 and P2 differred considerably in value, the use of the square root of their product is suggested for the rating. A similar but longer-term data analysis from a greater

number of existing stations in the region could shed more light into photochemical pollution status over the Mediterranean.

Optimisation of biomass liquefaction with glycerol and characterisation of the formed volatile products was described in (AL20).

Article (AL21) represents an investigation of the mycoremediation of lindane in liquid cultures of Pleurotus ostreatus and Hypoxylon fragiforme.

Boron biocides are one of the most frequently used components of commercial wood preservatives (AL27). They are very effective fungicides and insecticides, however they do not react with wood and thus leach from it in wet applications. In order to reduce leaching of boric acid, montan wax emulsion was introduced to the preservative solution. Spruce wood specimens were vacuum impregnated and afterwards leached according to the novel OECD and prCEN/TS 15119-1 procedures. Those two methods are non-continuous and are used for estimations of boron leaching from use class II and III applications. The results showed adding LGE emulsion does not reduce boron leaching significantly. Despite the fact that both methods applied are non-continuous, it can be evident, that OECD procedure is much more severe than the prCEN/TS 15119-1 one.

Boron biocides are most frequently used ingredients in commercial wood preservatives (AL29). They are very effective fungicides and insecticides, but they do not react with wood and thus leach from it in wet applications. This fact significantly limits the use of boron compounds in wood preservation. In order to reduce the leaching of boric acid, the emulsion of polyethylene (WE1) and an emulsion of oxidized polyethylene (WE6) wax were combined with boric acid (cB = 0.1% or 0.5% of boron). Spruce wood specimens were vacuum impregnated and afterwards leached according to the prCEN/TS 15119-1, ENV 1250-2 and EN 84 procedures. The results showed that boron leaching is predominantly influenced by moisture content of wood during leaching, and furthermore by the concentration gradient (frequency of water replacement). The fact that the prCEN/TS 15119-1 leaching procedure is less severe than the other two methods is also demonstrated in the results. The results of the EN 84 and ENV 1250 tests are comparable, while the results of the prCEN/TS 15119-1 testing are not in line with the other two methods. Considerable portions of boron are already leached from wood in the first leaching cycles. WE6 wax emulsion (oxidized polyethylene wax emulsion) in combination with heat treatment reduces boron leaching to a certain extent. On the other hand, impregnation of wood with WE1 (polyethylene wax emulsion) does not reduce it and it even enhances it.

Members of our programme group belong to academia and their primary task is education of undergraduate and graduate students and the production of highly trained specialists for chemical and related industries in Slovenia. The members of our group supervised 26 diploma theses in 2010 and supervised or co-supervised three master and seven doctoral theses and thus markedly contributed to the progress of chemical and pharmaceutical industries in our country.

SINTEZA, STRUKTURA, LASTNOSTI SNOVI IN MATERIALOV
SYNTHESIS, STRUCTURE AND PROPERTIES OF COMPOUNDS AND MATERIALS

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0175

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Ivan Leban

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
prof. dr. Jadran Maček
prof. dr. Stane Pejovnik
prof. dr. Ivan Leban
prof. dr. Boris Čeh
doc. dr. Mitja Robert Kožuh
prof. dr. Alojz Demšar
doc. dr. Klementina Zupan
doc. dr. Saša Petriček
prof. dr. Anton Meden
prof. dr. Iztok Turel
doc. dr. Amalija Golobič
doc. dr. Marjan Marinšek
doc. dr. Bojan Kozlevčar
dr. Nives Kitanovski
doc. dr. Andrej Pevec
doc. dr. Nina Lah
doc. dr. Franc Perdih
prof. dr. Primož Šegedin, v pokoju / retired

Mladi raziskovalci / Young Researchers
Marta Kasunič
Simona Medvešček
Katarina Stare
Jakob Kljun
Rosana Hudej
Maja Vidmar
Tina Prinčič

Strokovni sodelavec / Research Assistant
dr. Vojmir Francetič

Tehniki / Technicians
Aleš Knez
Vinko Volk

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Vsebino raziskovalnega programa lahko razdelimo v dva sklopa. Prvi sklop se ukvarja z osnovnimi raziskavami, drugi sklop pa naj bi bil bolj usmerjen v uporabne raziskave.

V okviru programa smo raziskovali pogoje priprave različnih spojin, anorganskih koordinacijskih in organokovinskih spojin z različnimi ligandi. Kemijsko čiste produkte smo karakterizirali z različnimi fizikalno-kemijskimi metodami in poskusili smo določati njihovo biološko učinkovitost. Podoben postopek smo uporabili pri materialih. Raziskovalni program je močno povezan s pedagoško usmeritvijo Katedre za anorgansko kemijo in Katedre za anorgansko tehnologijo in materiale, UL FKKT. Močno je poudarjeno sodelovanje z drugimi programskimi skupinami.

Za drugo leto raziskovalnega programa (2010) smo predvidevali nadaljevanje sintez in fizikalno-kemijsko karakterizacijo izoliranih spojin in materialov.

Povzetek pregleda iz baze podatkov SICRIS za to obdobje je v kategoriji izvirnih znanstvenih člankov 1.01 dalo 38 zadetkov, v kategoriji preglednih znanstvenih člankov 1.02 1 zadetek in v kategoriji kratkih znanstvenih prispevkov 1.03 3 zadetke.

OSREDNJE TEME PROGRAMA

Osrednje teme programa so večplastne. V okviru programske skupine smo se predvsem ukvarjali s koordinacijskimi spojinami, kinoloni, sintezo in karakterizacijo lantanoidnih kompleksov, različnimi strukturnimi raziskavami in novimi materiali.

V letu 2010 smo torej nadaljevali s sintezami in karakterizacijo novih spojin. Pripravili smo več novih spojin in jim določili kristalne strukture. Te spojine so: bakrovi kompleksi z nikotinamidom in isonikotinamidom, bakrovi halidni kompleksi ter kobaltova koordinacijska spo-

jino. Posebno zanimive so naslednje spojine: Zn(II) kompleks z DNA, rutenijevi kompleksi, platinovi(II) kompleksi ter kompleksi niklja z kinoloni. V sodelovanju s Krko d.d. smo določili strukture kokristalov flukonazola z različnimi kislinami. Določene so bile strukture različnim organskim spojinam. Študirali smo C-H interakcije, magnetne lastnosti fluorokobaltata(II), elektroporacijo rutenijevih(II) kompleksov in luminiscentne lastnosti Eu in Tb kompleksa.

V drugem delu smo bili uspešni pri rasti delcev določene velikosti ZnO in pri sintranju keramike NiO-YSZ.Pri slednjem je največja prednost te metode, da sta obe fazi NiO in YSZ v kompozitu naključno porazdeljeni na nanometrskem nivoju. Večina raziskav je bila objavljena v mednarodnih znanstvenih revijah. Vse podrobnosti so podane v besedilih prispevkov.

Iz bibliografskega pregleda se lahko razbere intenzivno sodelovanje z drugimi univerzami, raziskovalnimi inštituti v Sloveniji in v tujini.

To raziskovalno delo je bilo možno le z uporabo vrhunske raziskovalne opreme, s katero pa so določene težave, ko gre za vzdrževanje. Če bi bila oprema vključena v infrastrukturni center, teh težav ne bi bilo.

ZNANSTVENI DOSEŽKI

Omeniti velja zlasti naslednje dosežke po prostem izboru vodje programske skupine:

KARAKTERIZACIJA MIKROSTRUKTURE SINTRANIH PRAHOV NiO-YSZ PRIPRAVLJENIH Z ZGOREVALNO SINTEZO

Materiale na osnovi NiO-YSZ največ uporabljamo kot anode v visokotemperaturnih gorivnih celicah (SOFC). Materiale za izdelavo anod smo pripravili z zgorevalno sintezo iz citratno nitratnih gelov. Največja prednost te metode je, da sta obe fazi NiO in YSZ v kompozitu naključno porazdeljeni na nanometrskem nivoju. Razvoj mikrostrukture teh materialov smo zasledovali po sintranju tablet pri različnih temperaturah ter naknadni redukciji.

– MARINŠEK, Marjan, ZUPAN, Klementina. Microstructure evaluation of sintered combustion-derived fine powder NiO-YSZ, Ceram. Int., vol. 36, no. 3, str. 1075–1082, 2010, doi: 10.1016/j.ceramint.2009.12.014.

^{6}Li MAS NMR SPEKTROSKOPIJA IN »FIRST-PRINCIPLES« IZRAČUN KOT KOMBINIRANO ORODJE ZA RAZISKAVE POLIMORFIZMA Li_2MnSiO_4

V tem delu poročamo o razrešitvi težkega vprašanja polimorfnih oblik litijevega manganovega silikata, ki ima potencialno uporabo kot katodni material v litijevih akumulatorjih. Pri različnih pogojih sinteze in obratovanja akumulatorjev prihaja do različnih polimorfnih oblik, kar lahko povzroči precej spremenjene lastnosti katode. S kombinacijo različnih tehnik, kjer je naša skupina bistveno prispevala s strukturnimi študijami na osnovi praškovne difrakcije, je uspelo pojasniti polimorfne prehode in definirati pogoje nastanka različnih polimorfnih oblik.

– MALI, Gregor, MEDEN, Anton, DOMINKO, Robert. ^{6}Li MAS NMR spectroscopy and first-principles calculations as a combined tool for the investigation of Li_2MnSiO_4 polymorphs. Chem. commun. (Lond., 1996), 2010, issue 19, str. 3306–8, doi: 10.1039/c003065a.

INTERAKCIJE NIKELJ-KINOLONI. 3. DEL, KOMPLEKSI NIKLJA(II) Z ANTIBAKTERIJSKO UČINKOVINO FLUMEKIN

Pripravljene in okarakterizirane so bile nove koordinacijske spojine niklja(II) s kinolonsko antibakterijsko učinkovino flumekin v prisotnosti dušikovih heterocikličnih ligandov. Določene so bile strukture prvih kompleksov z flumekinom: bis(4-benzilpiridin)bis (flumekinato)nikelj, (2,2′-bipiridin)bis(flumekinato)nikelj in (1,10-fenantrolin)bis (flumekinato)nikelj. Kompetitivne študije z etidijevim bromidom, ciklična voltamografija in UV spektroskopija so pokazale, da se spojine močno vežejo na CT DNA in serumske proteine.

– SKYRIANOU, Kalliopi C., PERDIH, Franc, TUREL, Iztok, KESSISSOGLOU, Dimitris P., PSOMAS, George. Nickel-quinolones interaction. Part 3, Nickel(II) complexes of the antibacterial drug flumequine. *J. inorg. biochem.*. [Print ed.], 2010, vol. 104, no. 7, str. 740–749.

SINTEZE IN KRISTALNE STRUKTURE KOMPLEKSOV MANGANOVIH, NIKLJEVIH IN CINKOVIH KLORIDOV Z DIMETOKSIETANOM IN DI(2-METOKSIETIL)ETROM

Kompleksi enostavnih kovinskih kloridov so zelo primerna izhodna snov za sinteze koordinacijskih in organokovinskih spojin. Opisali smo sintezo in določili strukturo petih novih kompleksov manganovega, nikljevega in cinkovega klorida.

– PETRIČEK, Saša, DEMŠAR, Alojz. Syntheses and crystal structures of manganese, nickel and zinc chloride complexes with dimethoxyethane and di(2-methoxyethyl) ether, Polyhedron, vol. 29, no. 18, str. 3329–3334, 2010, doi: 10.1016/j.poly.2010.09.014.

KOKRISTALI FLUKONAZOLA Z DIKARBOKSILNIMI KISLINAMI

V sodelovanju s farmacevtsko družbo Krka d.d. smo raziskovali kokristalizacijo flukonazola – učinkovitega triazolnega antimikotika z različnimi farmacevtsko sprejemljivimi spojinami. Z metodo rentgenske strukturne analize smo določili kristalne strukture treh kokristalov z dikarboksilnimi kislinami: glutarno, fumarno in maleinsko kislino. Prisotnost farmacevtsko sprejemljive substance v trdnem namreč lahko bistveno izboljša kemijsko-fizikalne lastnosti učinkovine, v primeru flukonazola predvsem topnosti, ker je sam flukonazol v vodi zelo slabo topen.

– KASTELIC, Jože, HODNIK, Žiga, ŠKET, Primož, PLAVEC, Janez, LAH, Nina, LEBAN, Ivan, PAJK, Matjaž, PLANINŠEK, Odon, KIKELJ, Danijel. Fluconazole cocrystals with dicarboxylic acids, Cryst. growth des., vol. 10, no. 11, str. 4943–4953, 2010, doi: 10.1021/cg1010117.

DRUGI RELEVANTNI DOSEŽKI

SEVESO II DIREKTIVA V SLOVENIJI

Umestitev pomembne okoljevarstvene Seveso II direktive v slovenski prostor.

– KOŽUH, Mitja, The Seveso II Directive in New European Member States : the Case of Slovenia, Acta chim. slov., vol. 57, no. 1, str. 17–28, 2010, http://acta.chem-soc.si/57/57-1-017.

ENOSTAVNA PRIPRAVA OBETAVNIH LUMINISCENČNIH MATERIALOV NA OSNOVI KOORDINACIJSKIH SPOJIN LANTANOIDOV S PIKOLINSKO KISLINO

Iz lahko dostopnih in poceni reaktantov smo pripravili tri spojine s splošno formulo $[H_2N(Me)_2]_3[Ln(2,6\text{-}dpa)_3]$. Le-te se da pripraviti hitro in z visokim sinteznim izkoristkom (> 80 %) ob filtriranju reakcijske zmesi po eni uri segrevanja v DMF. Eu in Tb spojina sta bili strukturno okarakterizirani s pomočjo monokristalne difrakcije. Vse tri spojine imajo nenavadno visoke absorpcijske koeficiente in kvantne učinkovitosti ter so temperaturno obstojne ter odporne na vplive UV svetlobe in vode.

– MOOIBROEK, Tiddo Jonathan, GAMEZ, Patrick, PEVEC, Andrej, KASUNIČ, Marta, KOZLEVČAR, Bojan, FU, Wen-Tian, REEDIJK, Jan. Efficient, stable, tunable, and easy to synthesize, handle and recycle luminescent materials : [H[sub]2NMe[sub]2][sub]3[Ln(III)(2,6-dipicolinolate)[sub]3] (Ln = Eu, Tb, or its solid solutions). *Dalton trans. (2003. Print)*, 2010, vol. 39, no. 28, str. 6483–6847, doi: 10.1039/C000076K.

KEMIJSKE REAKCIJE

Učbenik kemije za drugi razred gimnazije.

– GODEC, Andrej, LEBAN, Ivan. Kemijske reakcije : učbenik za kemijo v gimnaziji. 1. izd. Ljubljana: Modrijan, 2010. 175 str., ilustr. ISBN 978-961-241-422-1.

ORGANIZACIJA IN PREDSEDOVANJE NA SLOVENSKO-HRVAŠKIH KRISTALOGRAFSKIH SREČANJIH – 19. SREČANJE STRUNJAN.

Organizacija in predsedovanje letnim tradicionalnim srečanjem z mednarodno udeležbo (60–80 udeležencev).

– Nineteenth Slovenian-Croatian Crystallographic Meeting, 18–20 June, 2010, Strunjan, Slovenia, LAH, Nina (ur.), LEBAN, Ivan (ur.). Book of abstracts [and] programme. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010. 67 str., ilustr.

RAZISKOVALNO-RAZVOJNA DEJAVNOST V SLOVENIJI

Diskusija o umestitvi centrov odličnosti v Sloveniji.

– Raziskovalno-razvojna dejavnost v Sloveniji LEBAN, Ivan. Prestrukturiranje raziskovalno-razvojne dejavnosti. V: GOLOB, Janvit (ur.), TRATNIK-VOLASKO, Marjeta (ur.). Kaj lahko pričakujemo od centrov odličnosti?, (Zbornik referatov in razprav, 2010, št. 1). Ljubljana: Državni svet Republike Slovenije, 2010, str. 21–23.

MEDNARODNO SODELOVANJE

– COST D39 (2007–2011): Ruthenium anticancer compounds (nosilec na FKKT I. Turel)
– Bilateralno sodelovanje z Avstrijo 2009–2010: Rutenijeve spojine in njihova možna uporaba v elektrokemoterapiji (nosilec I. Turel)

DRUGO SODELOVANJE

– Pogodba z Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika (J. Golob, B. Kozlevčar)
– Sodelovanje s Salonitom, Anhovo (A. Meden, J. Maček)
– Sodelovanje s Krko, Novo mesto (A. Meden, N. Lah, I. Leban)

PROMOCIJA ZNANOSTI

– Noč znanstvenic in znanstvenikov 2010 (A. Knez, V. Francetič, I. Leban)
http://abra.fkkt.uni-lj.si/fn01leban/rn2010/
– 9. Unescov naravoslovni tabor 2010, Osn. šola Griže (A. Knez, I.Leban)
– BEST dnevi tehnike 2010 (A. Knez, I.Leban)
– 3. festival naravoslovja HOKUS POKUS 2010, Pionirski Dom (A. Knez, I. Leban)

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

Our programme is divided into fundamental research and applied research and focuses on studies of various new compounds, i.e. inorganic, coordination and organometallic. Chemically pure product were characterized by various physico-chemical methods and also some biological activities were tested. Similar procedures were used with new materials. The whole research programme is closely linked with pedagogical work of the Chair of Inorganic Chemistry and the Chair of Inorganic Chemical Technology and Materials (University of Ljubljana, Faculty of Chemistry and Chemical Technology). There is an extensive collaboration with other research groups.

The plan for the second year (2010) was continuing the research on the synthesis and physico-chemical characterization of the compounds and new materials.

In 2010 the SICRIS database registered 38 contributions for the category – original scientific paper (1.01), 1 paper in the category – review paper (1.02) and 3 papers in the category of short scientific article (1.03).

RESEARCH TOPICS

There have been several fields of interest in our programme group. These involve: studying coordination compounds, quinolones, complexes of lanthanide halides, various structural work and new materials.

In the year 2010 new chemical compounds were synthetised and characterised. The obtained crystals were subjected to X-ray structural analysis.

The following interesting compounds were prepared: copper complexes with nicotineamide and isonicotineamide, copper halide complexes and cobaltous complex compound. The compounds of special interest were: Zn(II) complex with DNA, ruthenium complexes, platinum(II) complexes and nickel complexes with quinolones. In collaboration with the com-

pany Krka d.d. we determined crystal structures of cocrystals of fluconazole with different acids. Several organic crystal structures were also determined. Furthermore, the study on C-H interactions, magnetic properties of fluorocobaltate(II), electroporation of ruthenium(II) complexes and luminiscent properties of Eu and Tb complexes was performed.

We were successful in the growing of ZnO particlec and sintering of the NiO-YSZ ceramics. The main advantage of the preparation method used was reflected in the fact that after the synthesis both, NiO and YSZ phases were randomly distributed on a nanometer scale. Most of the research was published in international journals. All details are documented in scientific articles.

Bibliographic data reflect an extensive collaboration of our research group with various universities and research institutes in Slovenia and abroad.

Our research could not have been made without up-to-date research equipment. However, we have experienced some difficulties with the maintenance of the equipment.

SCIENTIFIC ACHIEVEMENTS

The following achievements need to be highlighted:

MICROSTRUCTURE EVALUATION OF SINTERED COMBUSTION-DERIVED FINE POWDER NiO-YSZ.

NiO-YSZ based cermets are the most widely adopted materials for SOFC anodes. Citrate-nitrate combustion synthesis was used for the preparation of NiO-YSZ. The main advantage of the preparation method used was the fact that after the synthesis both phases NiO and YSZ were randomly distributed on a nanometer scale. NiO-YSZ powder composites were shaped, sintered at different temperatures and reduced to Ni-YSZ and subsequently submitted to microstructure investigations.

– MARINŠEK, Marjan, ZUPAN, Klementina. »Microstructure evaluation of sintered combustion-derived fine powder NiO-YSZ«, Ceram. int., Vol. 36, No. 3, p.p. 1075–1082, 2010, doi: 10.1016/j.ceramint.2009.12.014.

^{6}Li MAS NMR SPECTROSCOPY AND FIRST-PRINCIPLES CALCULATIONS AS A COMBINED TOOL FOR THE INVESTIGATION OF Li_2 $MnSiO_4$ POLYMORPHS

In this work we propose a solution to a difficult problem of polymorphism of lithium manganese silicate. The material is potentially applicable as cathode material in rechargeable lithium batteries. Different synthesis and working conditions resulted in various polymorphjic forms, which can cause some changes in the properties of the cathode. A combination of various methods leads to the clarification of polymorph transitions and to the definition of conditions leading to defined polymorphic forms. Our group has essentially contributed to the results on structural studies, based on powder diffraction.

– MALI, Gregor, MEDEN, Anton, DOMINKO, Robert. ^{6}Li MAS NMR spectroscopy and first-principles calculations as a combined tool for the investigation of Li_2MnSiO_4 polymorphs. Chem. commun. (Lond., 1996), 2010, issue 19, str. 3306–8, doi: 10.1039/c003065a.

NICKEL-QUINOLONES INTERACTION. PART 3, NICKEL(II) COMPLEXES OF THE ANTIBACTERIAL DRUG FLUMEQUINE

Nickel(II) complexes with the quinolone antibacterial agent flumequine in the presence of nitrogen donor heterocyclic ligands were synthesized and structurally characterized. The crystal structures of the first flumequinato complexes were reported: bis(4-benzylpyridine) bis(flumequinato)nickel, (2,2′-bipyridine)bis(flumequinato)nickel and (1,10-phenanthroline) bis(flumequinato)nickel. Competitive studies with ethidium bromide, the cyclic voltammograms and UV study have shown that the complexes bind strongly to CT DNA and to serum albumin protein.

– SKYRIANOU, Kalliopi C., PERDIH, Franc, TUREL, Iztok, KESSISSOGLOU, Dimitris P., PSOMAS, George. Nickel-quinolones interaction. Part 3, Nickel(II) complexes of the antibacterial drug flumequine. *J. inorg. biochem.*. [Print ed.], 2010, Vol. 104, No. 7, p.p. 740–749.

SYNTHESES AND CRYSTAL STRUCTURES OF MANGANESE, NICKEL AND ZINC CHLORIDE COMPLEXES WITH DIMETHOXYETHANE AND DI(2-METHOXYETHYL) ETHER.

Complexes of metal chlorides are useful starting compounds for syntheses of coordination and organometalic compounds. We have reported on the syntheses and structures of five novel manganese, nickel and zinc chloride complexes.

– PETRIČEK, Saša, DEMŠAR, Alojz. Syntheses and crystal structures of manganese, nickel and zinc chloride complexes with dimethoxyethane and di(2-methoxyethyl) ether, Polyhedron, Vol. 29, No. 18, p.p. 3329–3334, 2010, doi: 10.1016/j.poly.2010.09.014.

FLUCONAZOLE COCRYSTALS WITH DICARBOXYLIC ACIDS

In collaboration with the pharmaceutical company Krka d.d. we have investigated the cocrystalization of fluconazole: a wide spectrum triazole antifungal agent was used in the treatment of localized candidiasis and systematic therapy of candidial infections, dermatophytic fungal infections and cryptococcal meningitis. This agent is commonly used as accompanying therapy for immunodeficient patients with AIDS or cancer and patients taking immunodepresive agents. It is only slightly soluble in water. Along these lines we have focused our research to the preparation of new fluconazole cocrystals.

– KASTELIC, Jože, HODNIK, Žiga, ŠKET, Primož, PLAVEC, Janez, LAH, Nina, LEBAN, Ivan, PAJK, Matjaž, PLANINŠEK, Odon, KIKELJ, Danijel. Fluconazole cocrystals with dicarboxylic acids, Cryst. growth des., Vol. 10, No. 11, p.p. 4943–4953, 2010, doi: 10.1021/cg1010117.

OTHER RELEVANT ACHIEVEMENTS

SEVESO II DIRECTIVE IN SLOVENIA

Application of Environmental Protection Directive Seveso II in Slovenia.

– KOŽUH, Mitja, The Seveso II Directive in New European Member States : the Case of Slovenia, Acta chim. slov., Vol. 57, No. 1, p.p. 17–28, 2010, http://acta.chem-soc.si/57/57-1-017.

AN EASY WAY TO SYNTHESIZE PROMISING LUMINESCENT MATERIALS ON THE BASIS OF COORDINATION COMPOUNDS OF LANTHANOIDS WITH PICOLINIC ACID

Three compounds with the general formulae $[H_2N(Me)_2]_3[Ln(2,6\text{-}dpa)_3]$ were prepared from cheap and readily available reactants. Microcrystalline compounds were isolated in high yields (> 80%) by simple filtration, after only one hour reaction time in refluxing DMF. The Eu and Tb compounds were structurally characterized by single crystal X-ray diffraction. The compounds have unusual high-absorption coefficients and quantum efficiencies. Furthermore, they are thermally stable and appear to be UV and water tolerant.

– MOOIBROEK, Tiddo Jonathan, GAMEZ, Patrick, PEVEC, Andrej, KASUNIČ, Marta, KOZLEVČAR, Bojan, FU, Wen-Tian, REEDIJK, Jan. Efficient, stable, tunable, and easy to synthesize, handle and recycle luminescent materials : [H[sub]2NMe[sub]2][sub]3[Ln(III)(2,6-dipicolinolate)[sub]3] (Ln = Eu, Tb, or its solid solutions). *Dalton trans. (2003. Print)*, 2010, Vol. 39, No. 28, p.p. 6483–6847, doi: 10.1039/C000076K.

CHEMICAL REACTIONS

Course-book for second year chemistry courses in grammar schools.

– GODEC, Andrej, LEBAN, Ivan. Kemijske reakcije : učbenik za kemijo v gimnaziji. 1. izd. Ljubljana: Modrijan, 2010. 175 pp., illustr. ISBN 978-961-241-422-1.

SLOVENIAN-CROATIAN CRYSTALLOGRAPHIC MEETINGS – 19TH SLOVENIAN-CROATIAN CRYSTALLOGRAPHIC MEETING, STRUNJAN

Organisation and chairing of traditional meetings with the international participation (60–80 crystallographers).

– Nineteenth Slovenian-Croatian Crystallographic Meeting, 18–20 June, 2010, Strunjan, Slovenia, LAH, Nina (Ed.), LEBAN, Ivan (Ed.). Book of abstracts [and] programme. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010. 67 pp., illustr.

R&D ACTIVITY IN SLOVENIA

Discussion about the position of the Centers of Excellence (CoE) in small countries like Slovenia.

– Raziskovalno-razvojna dejavnost v Sloveniji LEBAN, Ivan. Prestrukturiranje raziskovalno-razvojne dejavnosti. V: GOLOB, Janvit (ur.), TRATNIK-VOLASKO, Marjeta (ur.). Kaj lahko pričakujemo od centrov odličnosti?, (Zbornik referatov in razprav, 2010, No. 1). Ljubljana: Državni svet Republike Slovenije, 2010, p.p. 21–23.

INTERNATIONAL COOPERATION

– COST D39 (2007–2011): Ruthenium anticancer compounds (Principal researcher: I. Turel).
– Bilateral cooperation with Austria (2009–2010): Ruthenium compounds and their possible applications in electrochemotherapy (Principal researcher: I. Turel)

OTHER COOPERATION

– Contract with Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika (J. Golob, B. Kozlevčar)
– Cooperation with Salonit d.d., Anhovo (A. Meden, J. Maček)
– Cooperation with Krka d.d., Novo mesto (A. Meden, N. lah, I. Leban)

PROMOTION OF SCIENCE

– Researchers' Night 2010 (A. Knez, V. Francetič, I. Leban)
http://abra.fkkt.uni-lj.si/fn01leban/rn2010/
– 9th UNESCO Natural-Sciences Camp 2010, Primary School Griže (A. Knez, I. Leban)
– BEST Technology Days 2010 (A. Knez, I. Leban)
– 3rd Festival of Natural Sciences HOKUS POKUS 2010, Pionirski Dom (A. Knez, I. Leban)

SINTEZE IN TRANSFORMACIJE ORGANSKIH SPOJIN. NOVI REAGENTI V STEREOSELEKTIVNI IN REGIOSELEKTIVNI SINTEZI AMINOKISLIN KOT INTERMEDIATOV V ORGANSKI SINTEZI

SYNTHESES AND TRANSFORMATIONS OF ORGANIC COMPOUNDS. NEW REAGENTS IN STEREOSELECTIVE AND REGIOSELECTIVE SYNTHESIS OF AMINO ACIDS AS INTERMEDIATES IN ORGANIC SYNTHESIS

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0179

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

akademik prof. dr. Branko Stanovnik

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
akad. prof. dr. Branko Stanovnik
prof. dr. Jurij Svete
dr. Uroš Uršič
dr. Jernej Wagger

Mladi raziskovalci / Young Researchers
Jernej Baškovč
Jure Bezenšek
Črt Malavašič
Ana Novak

Tehniki / Technicians
Tončka Kozamenik
Tatjana Stipanovič

POROČILO O REALIZACIJI PROGRAMA

OSREDNJE TEME PROGRAMA TER ZNANSTVENI IN DRUGI RELEVANTNI DOSEŽKI

V okviru programa P1–0179 smo študirali nove sintezne metode in pristope za pripravo funkcionaliziranih heterocikličnih spojin, ki vsebujejo terpensko, etilaminsko, amino kislinsko, dipeptidno, amino alkoholno in sorodne strukturne enote. Naša metodologija je vključevala predvsem sintezne pristope, ki temeljijo na primarni pripravi ustrezno funkcionaliziranih (acikličnih) prekurzorjev, ki ji nato sledi gradnja heterocikličnega obroča kot ključni korak sinteze ciljnega tipa spojin. Priprava prekurzorjev je temeljila na pretvorbi komercialno dostopnih izhodnih spojin po literaturnih postopkih oziroma po lastnih postopkih, temelječih na splošnih principih organske sinteze. Za gradnjo heterocikličnih sistemov pa smo uporabljali predvsem dve splošni metodologiji:

a) ciklokondenzacije reagentov enaminonskega tipa z različnimi dinukleofili
b) [2+2], [3+2] in [4+2] cikloadicije, zlasti 1,3-dipolarne cikloadicije azometin iminov na različne acetilene in olefine.

Pomembni rezultati raziskovalnega dela so bili doseženi na naslednjih področjih:

1. Nove metode za sintezo funkcionaliziranih heterocikličnih spojin
2. Nove metode in reagenti v stereoselektivni in asimetrični sintezi
3. Kombinatorna sinteza heterocikličnih spojin
4. Sinteza novih heterocikličnih sistemov

Rezultati vseh raziskav so bili objavljeni v mednarodnih znanstvenih časopisih z IF. Prav tako smo o njih poročali na mednarodnih kongresih in simpozijih. O pomenu dosedanjih raziskav pričajo povabila za plenarna in vabljena predavanja po svetu in predavanja na raznih univerzah, vabila za pisanje preglednih člankov oziroma poglavij v mednarodno priznanih revijah in knjigah.

(2E,3Z)-2-(1-Metil-2,5-dioksoimidazolidin-4-iliden)-3-[(arilamino- ali heteroarilamino)metilen]sukcinat, ki nastane pri [2+2]cikloadiciji (5Z)-5-[(dimetilamino)metilen]-3-metilimidazolidin-2,4-diona in dimetil acetilendicarboksilata s sledečo substitucijo dimetulaminske skupine z aromatskimi ali heteroaromatskimi amini, daje pri segrevanju v etanolu v prisotnosti kalijevega hidroksida kalije soli intermediata, ki ob nakisanju s solno kislino dajo derivate (E)- in (Z)- metil4-(2-hidroksi-1-metil-5-okso-1H-imidazol-4(5H)-iliden)-5-okso-1-fenil-4,5-dihidro-1H-pirol-3-karboksilata, medtem ko nastanejo pri alkiliranju derivati novega triazafulvalenskega sistema. (URŠIČ, Uroš, SVETE, Jurij, STANOVNIK, Branko. *Tetrahedron* 2010, *66*, 4346–4356).

Študirali smo [2+2]cikloadicije (*E*)-3-dimetilamino-1-heteroaril-prop-2-en-1-onov na dimetil acetilendikarboksilat pod vplivom mikrovalov. Pri tem nastanejo (2*E*,3*E*)-dimetil-2-[(dimetilamino)metilen]-3-(substituirani)sukcinati v 8–91 % izkoristku. Pri cikloadiciji metil

acetilendikarboksilata na (*E*)-1-(4,5-dihidrotiazol-2-il)-3-(dimetilamino)prop-2-en-1-on pa poteče bistveno drugače, tako da nastane poleg normalnega produkta še (*E*)-dimetil 6-[2-(dimetilamino)vinil]-5-okso-2,3,5,7a-tetrahidropirolo[2,1-*b*]tiazol-7,7a-dikarboksilat v 32 % izkoristku. Uspeli smo razložiti tudi mehanizem te reakcije. [2+2]Cikloadicija poteče najprej na endociklično C=N vez, ki ji sledita dve 1,3-sigmatropni premestitvi, razširitev štiričlenskega obroča v petčlenski obroč in premestitev metilne skupine. (BEZENŠEK, Jure, KOLEŠA, Tanja, GROŠELJ, Uroš, WAGGER, Jernej, STARE, Katarina, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. *Tetrahedron Letters* 2010, *51*, 3392–3397).

Po enaminonski metodologiji smo sintetizirali tudi dva N-benzilirana analoga antioksidanta alkaloida neoehinulina A v racemni obliki. (WAGGER, Jernej, GROŠELJ, Uroš, SVETE, Jurij, STANOVNIK, Branko. *Synlett* 2010, 1197–1200).

Pripravili smo knjižnico dvanajstih N(4´)-substituiranih di-t-butil (2S,4E)-4-arilaminometiliden-5-oksopirolidin-1,2-dikarboksilatov z 47–90 % izkoristkom s paralelno s kislino katačizirano sintezo iz di-t-butil (2S,4E)-4-dimetilaminometiliden-5-oksopirolidin-1,2-dikarboksilatov in anilinov, etil glicinata in etil alaninata. Konfiguracija okrog dvojne vezi je bila določena z NMR metodami. **(**SVETE, Jurij, GROŠELJ, Uroš, BAŠKOVČ, Jernej, DAHMANN, Georg, STANOVNIK, Branko. *Z. Naturforsch*. 2010, *65b*, 811–820).

Razvili smo tri sintezne metode za pripravo 1,5-disubstituiranih 1,5,6,7-tetrahydro-4*H*--pirazolo[4,3-*c*]piridin4-onov kot heterocikličnih analogov histamine. Pri prvi metodi smo izhajali iz metil 5-(2-aminoetil)-1*H*-pirazol-4-karboksilatov, ki smo jih N-alkilirali in tako pripravljene sekundarne amine ciklizirali v bazičnem v končne produkte s 17–92 % izkoristkom. Po drugi metodi smo najprej ciklizirali v pirazolo[4,3-*c*]piridin-4-one nesubstituirane na mestu 5, nato pa jih benzoilirali do končnih produktov s 36–49 % izkoristkom. Tretja metoda je šeststopenjska pretvorba metil akrilata v 1-benzilpiperidin-2,4-dione, ki ji sledi reakcija z *N*,*N*-dimetilformamid dimetilacetalom (DMFDMA) in ciklizacija enaminona v kislem s metil-, fenil- in *tert*-butilhidrazinom do končnega produkta v 79–87 % izkoristkom. (ŽEROVNIK, Darja, GROŠELJ, Uroš, KRALJ, David, MALAVAŠIČ, Črt, BEZENŠEK, Jure, DAHMANN, Georg, STARE, Katarina, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. *Synthesis* 2010, 3363–3373).

Ugotovili smo, da pri kondenzaciji malononitrila z dialkil aceton-1,3-dikarboksilatom nastanejo alkil (3-ciano-6-alkoksi-2-okso-1,2-dihidropiridin-4-il)acetate v nasprotju z literaturnimi podatki ko naj bi nastal dietil 3-(dicianometilen)glutarat. Pri nadaljni reakciji z DMFDMA nastanejo ustrezni (*E*)-alkil 2-(3-ciano-6-alkoksi-2-okso-1,2-dihidropiridin-4-il)-3-(dimetilamino) propenoati. (ŠIMUNEK, Petr, BAŠKOVČ, Jernej, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK**,** Branko**.** *Z. Naturforsch*. 2010, *65b*, 807–810).

Sintetizirane so bile PF_6 soli 5-benzil-1-izopropiliden- in 5-benzil-1-cinamiliden-3-metilimidazolidin-4-onov z različnimi substituenti na položaju *C*(2) in 14 takih spojin je dalo monokristale primerne za rentgensko strukturno analizo. Pri devetih strukturah leži fenilni obroč benzilne skupine nad heterocikličnim obročem v kontaktu s *cis*-substituentom na mesti *C*(2) (zamaknjena konformacija A); v treh primerih leži fenilni obroč benzilne skupine nad iminijevo π-ravnino (zamaknjena konformacija B); v dveh strukturah pa ima benzilna C-C vez poravnano konformacijo, ki postavi fenilni obroč maksimalno stran od svojih sosedov, to je C=O skupine, N=C-π-sistema in *cis*-substituenta na mestu *C*(2) heterocikličnega obroča. Kvalitativna konformacijska analiza vseh treh zamaknjenih konformacij benzilne C-C vezi kaže na neugodne sterične interakcije tako, da se poravnana konformacija kaže kot izhod iz te zagate. Najsodobnejše kvantno-kemijske metode, z velikim AO baznim setom (blizu limite) za točkovne izračune so bile uporabljene za izračun sedem od 14 iminijevih ionov, ki so v dveh zamaknjenih konformacijah A in B, z benzilno skupino nad obročem in nad iminijevim π-sistemom. Pri

vseh primerih se je izkazala kot najbolj stabilna izračunana konformera tista, ki je bila najdena tudi v kristalu. Razlike v energiji med konformerama so majhne (≤ 2 kcal/mol) kar skupaj z izračunano potencialno krivuljo za rotacijo okoli benzilne C-C vezi nakazuje, da benzilna skupina pri sobni temperaturi bolj ali manj prosto rotira. Pokazana je bila pomembnost intramolekularnih *London*-ovih disperzijskih sil (benzenov obroč v kontaktu s *cis*-substituentom pri konformaciji A) za DFT in ostale kvantno kemijske izračune; benzil-imidazolidinoni so se izkazali kot idealen sistem za detekcijo disperzijskih prispevkov med benzenovim obročem in alkil ali aril CH skupino. Enilidenski ioni tega tipa so reaktivni intermediati pri enantioselektivnih organokataliziranih konjugativnih adicijah, *Diels-Alder* reakcijah, in mnogih drugih transformacijah ki vključujejo *α,β*-nenasičene karbonilne spojine. Naši eksperimentalni in teoretični izračuni so diskutirani z vidika učinkovitosti 5-benzil-imidazolidinonov kot enentioselektivnih katalizatorjev. (SEEBACH, Dieter, GROŠELJ, Uroš, SCHWEIZER, W. Bernd, GRIMME, Stefan, MÜCK-LICHTENFELD, Christian. *Helvetica Chimica Acta* 2010, *93*, 1).

Strukture iminijevih soli, pripravljenih iz derivatov diarilprolinola ali imidazolidinona in *α,β*-nenasičenih aldehidov, so bile študirane z rentgensko praškovno difrakcijo, rentgensko strukturno analizo monokristalov, NMR spektroskopijo in DFT izračuni. Skoraj vse iminijeve soli tega tipa obstajajo v raztopini kot diastereoizomerne zmesi z (*E*)- in (*Z*)-konfiguracijo okoli +N=C dvojne vezi. Pri tej študiji so bila opažena (*E*)/(*Z*) razmerja od 88 : 12 do 98 : 2 in (*E*)/(*Z*) interkonverzije. Relativne hitrosti tvorbe (*E*)- in (Z)-izomerov iz amonijevih soli in *α,β*-nenasičenih aldehidov se razlikujejo od hitrosti vzpostavitve (*E*)/(*Z*)-ravnotežja v vsaj dveh primerih; več (*Z*)-izomera se tvori kinetično, kot ga najdemo kasneje po vzpostavi (*E*)/(*Z*)-ravnotežje. Glede na to, da stereoselektivne pretvorbe dobljene z mediacijo organokatalizatorjev tega tipa pogosto presegajo d.e. > 99 : 1, (*E*)-iminijevi intermediati verjetno reagirajo z nukleofili hitreje kot ustrezni (*Z*)-iminijevi intermediati. V članku se razglabljajo možni razlogi zakaj so (*E*)-iminijevi ioni bolj reaktivni kot (*Z*)-iminijevi ioni in zakaj se (*Z*)-iminijevi ioni tvorijo preferenčno pod kinetičnimi pogoji. Navedeni so tudi sorodni DFT izračuni. (SEEBACH, Dieter, GILMOUR, Ryan, GROŠELJ, Uroš, DENIAU, Gildas, SPARR, Christof, EBERT, Marc-Olivier, BECK, Albert. K, McCUSKER, Lynne B., ŠIŠAK, Dubravka, UCHIMARU, Tadafumi. *Helvetica Chimica Acta* 2010, *93*, 603).

PREGLEDNI ZNANSTVENI ČLANEK

V preglednem članku z naslovom **Dialkyl Acetone-1,3-Dicarboxylates and their Mono- and bis(Dimethylamino)methylidene Derivatives in the Synthesis of Heterocyclic Systems** smo opisali transformacije dialkil aceton-1,3-dicarboksilatov in njihovih (dimetilamino)metilidenskih derivatov: sinteze 1-substituiranih 4-etoksikarbonil-5-(etoksikarbonilmetil)pirazolov, sintezo pirazolo[4,3-*c*]piridinov, sinteze pirazolo[4,3-*d*][1,2]diazepinov, sinteze kondenziranih pirazol-3-il-pyrimidinov in kondenziranih pirazol-3-il-piranonov, pirazolo[1,5-*c*]pirimidin-5-onov, piridin-4(1*H*)-onov, 4-hidroksipiridin-2(1*H*)-onov in pirano[3,2-*c*]pridinonov, tiazolo[5,4-*c*]piridinov, 4-okso-1,4-dihidropiridazin-3,5-dikarboksilatov, heteroaril substituiranih pirimidinov, pirido[1,2-*a*]pirimidin-3-il)tiazol-5-karboksilatov in paralelno »solution-phase« sintezo of 1,4-dihidropiridinov. (STANOVNIK, Branko, GROŠELJ, Uroš. *Adv. Heterocycl. Chem.* 2010, *100*, 145-174).

OBJAVLJENO PLENARNO PREDAVANJE

V plenarnem predavanju z naslovom **From β-dimethylamino-α-acylamino-α,β-didehydro acid derivatives and related enaminones *via* heterocycles and heterocyclic amino acids to**

indole alkaloids so opisane sinteze naravnih spojin in njihovih analogov z enaminonsko metodologijo, to je aplisinopsinov in njihovih analogov, heteroarilindolov in policikličnih analogov meridianina ter analogov z uracilovo strukturno enoto, kondenziranih 3-(1*H*-indol-3-uil)-2*H*--piran-2-onov, dipodazinov in njihovih analogov, triprostatinov in drugih. (STANOVNIK, Branko. [plenary lecture]. V: KARTSEV, Viktor Georgievich (ur.). The Fourth International Conference CBC2010, August 2–6, 2010, Saint-Petersburg. *Sovremenye aspekty himii geterociklov : himija i biologičeskaja aktivnost sintetičeskih i prirodnyh soedinenij*. Moscow: ICSPF (International Charitable Scientific Partnership Foundation), 2010, str. 161–171).

SODELOVANJE S TUJIMI UNIVERZAMI IN DRUGIMI INSTITUCIJAMI

1. Zelo uspešno sodelovanje s skupino prof. dr. O. A. Attanasija z univerze v Urbinu (Italija) na področju reakcij 3-dimetilaminopropenoatov in sorodnih enaminonov in 1,2-diaza-1,3-butadienov (Vodja: B.Stanovnik)
2. Sodelovanje s prof. dr. W. Kantlehnerjem z univerze v Stuttgartu (Nemčija) na področju amid acetalov in sorodnih spojin kot reagentov v organski sintezni kemiji (Vodja: B. Stanovnik)
3. Sodelovanje s prof. dr. G. Maasom z univerze v Ulmu (Nemčija) na področju amid acetalov in sorodnih spojin kot reagentov v organski sintezni kemiji (Vodja: B. Stanovnik)
4. Zelo aktivno sodelovanje na področju sinteze heterocikličnih spojin s farmacevtsko tovarno BOEHRINGER-Biberach, Ingelheim (Nemčija) (Vodja: J. Svete)

MEDNARODNO PRIZNANJE

B. Stanovnik: Zlati znak (Gold Badge) Fundacije za mednarodno znanstveno partnerstvo za prispevek k svetovni znanosti in mednarodnemu znanstvenemu sodelovanju (Sankt Peterburg 2010)

DRUGA PRIZNANJA

B. Stanovnik: Priznanje Krke d.d. ob 40-letnici Krkinih nagrad za izjemen prispevek pri usmerjanju in spodbujanju mladih k raziskovalnemu delu

ČLANSTVO V MEDNARODNIH ZNANSTVENIH ODBORIH KONGRESOV IN SIMPOZIJEV IN DRUGE ADMINISTRATIVNE FUNKCIJE

B. Stanovnik:

a) Member of the Scientific Committee, European Colloquia of Heterocyclic Chemistry
b) Member of the Scientific Committee, Blue Danube Symposia of Heterocyclic Chemistry
c) Member of the Board of Electronic Journal ARKIVOC, Scientific Editor of ARKIVOC
d) Member of the Advisory Board, Advances in Heterocyclic Chemistry
e) Member of the Scientific Committee, TRAMECH Transmediterranean Symposia on Heterocyclic Chemistry
f) Member of International Advisory Committee of the IBN SINA InternationalConferences on Pure and Applied Heterocyclic Chemistry

g) Member of the Advisory Board, Trends in Heterocyclic Chemistry
h) Predstojnik Oddelka za mednarodno sodelovanje in znanstveno koordinacijo Slovenske akademije znanosti in umetnosti, Ljubljana, Slovenija
i) Dekan razreda za naravoslovne znanosti Evropske akadmije znanosti in umetnosti, Salzburg, Austria in legat EASA za Slovenijo za obdobje 2010–2014
j) Member of the Advisory Board, Croatica Chemica Acta
k) Member of the Advisory Editorial Board, Journal of Heterocyclic Chemistry
l) 1998–2004 Member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons, Den Haag, The Netherlands

RESEARCH PROGRAMME REPORT

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

Within the framework of the P1-0179 programme, novel synthetic methods and approaches for the preparation of heterocycles functionalized with terpene, ethylamine, amino acid, dipeptide, amino alcohol, and related structural elements were studied. Our methodology included synthetic approaches based on primary preparation of suitably functionalized (acyclic) precursors from commercially available starting materials, followed by heterocyclization as the key-step of the synthesis. Two general methods were used for the construction of the heterocyclic rings:

a) cyclocondensations of enaminone-type reagents with various dinucleophiles and
b) [2+2], [3+2] and [4+2] cycloadditions, with emphasis on 1,3-dipolar cycloadditions of azomethine imines on various acetylenes and olefins.

Within this context, the following achievements can be pointed out:

1. New methods for the synthesis of functionalized heterocyclic compounds:
2. New methods and reagents in stereoselective and asymmetric sysnthesis
3. Combinatorial synthesis of heterocyclic compounds
4. Synthesis of new heterocyclic systems

All the reseach results mentioned above have been published in international scientific journals with IF. The results were also presented in plenary and invited lectures at international meetings and various universities, as well as reported in review articles chapters in books.

(2*E*,3Z)-2-(1-methyl-2,5-dioxoimidazolidin-4-ylidene)-3-[(arylamino- or heteroarylamino)methylene]succinate obtained by [2+2] cycloaddition of (5*Z*)-5-[(dimethylamino)methylene)]-3-methylimidazolidine-2,4-dione and dimethyl acetylen edicarboxylate followed by substitution of the dimethylamino group with aromatic or heteroaromatic aminesgives potassium salts after heating in ethanol in the presence of potassium hydroxide,. Acidification with hydrochloric acid afforded mixtures of (*E*-)- and (*Z*)-isomers of methyl 4-(2-hydroxy-1-methyl-5-oxo-1*H*-imidazol-4(5*H*)-ylidene)-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrrole-3-carboxylates. On the other hand, alkylation with methyl iodide or benzyl bromide produced the corresponding methyl (*E*)-4-(2-methoxy- or 2-benzyloxy-1-methyl-5-oxo-1*H*-imidazol-4(5*H*)-ylidene)-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrrole-3-carboxylates, derivatives of a new triazafulvalene system. **(**URŠIČ, Uroš, SVETE, Jurij, STANOVNIK, Branko. *Tetrahedron* 2010, *66*, 4346–4356).

Microwave-assisted [2+2] cycloadditions of (*E*)-3-dimethylamino-1-heteroaryl-prop-2-en-1-ones to dimethyl acetilenedicarboxylates gave (2*E*,3*E*)-dimethyl-2-[(dimethylamino) methylene]-3-(substituted)succinates with 16–91% yield. In the case of 4,5-dihydrothiazoline derivative cycloaddition took place also to the endocyclic C=N double bond. The cycloaddition of (*E*)-1-(4,5-dihydrothiazol-2-yl)-3-(dimethylamino)prop-2-en-1-one, prepared from 1-(4,5-dihydrothiazol-2-yl)ethanone (**12b**) and DMFDMA, to DMAD, under microwave irradiation, afforded a mixture of the corresponding [2+2] cycloadduct in 8% yield and (*E*)-dimethyl 6-[2-(dimethylamino)vinyl]-5-oxo-2,3,5,7a-tetrahydropyrrolo[2,1-*b*]thiazole-7,7a-dicarboxy-late in 32% yield. We rationalize the formation of the latter compound by initial [2+2] cycloaddition of DMAD to the endocyclic C=N double bond to form the cycloadduct, followed by a serries of 1,3-sigmatropic shifts to finally arrive at the final product. (BEZENŠEK, Jure, KOLEŠA, Tanja, GROŠELJ, Uroš, WAGGER, Jernej, STARE, Katarina, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. *Tetrahedron Letters* 2010, *51*, 3392-3397).

Using enaminone methodology, two *N*-benzylated analogues of antioxidant, radical scavenging and neuroprotective neoechinuline A alkaloid were prepared. Since stereochemistry, according to SAR studies, does not play an important role, both analogues were prepared in racemic form. (WAGGER, Jernej, GROŠELJ, Uroš, SVETE, Jurij, STANOVNIK, Branko. *Synlett* 2010, 1197–1200).

A library of twelve *N*(4′)-substituted di-*tert*-butyl (2*S*,4*E*)-4-arylaminomethylidene-5-oxopyrrolidine-1,2-dicarboxylates were prepared with the yield of 47–90% by parallel acid-catalysed treatment of di-*tert*-butyl (2*S*,4*E*)-4-[(dimethylamino)methylidene]-5-oxopyrrolidine-1,2-dicarboxylate with anilines, ethyl glycinate, and ethyl β -alaninate. Acidolytic deprotection afforded the corresponding (2*S*,4*E*)-4-arylaminomethylidene-5-oxopyrrolidine-2-carboxylic acids with 39 – 99% yield. The configuration around the C=C double bond in the enaminones and was determined by NMR spectroscopy. **(**SVETE, Jurij, GROŠELJ, Uroš, BAŠKOVČ, Jernej, DAHMANN, Georg, STANOVNIK, Branko. *Z. Naturforsch*. 2010, *65b*, 811-820).

Three synthetic methods for the preparation of 1,5-disubstittued 1,5,6,7-tetrahydro-4*H*-pyrazolo[4,3-*c*]pyridine-4-ones as heterocyclic histamine analogues were developed. The first method starts from easily available methyl 5-(2-aminomethyl)-1*H*-pyrazole-4-carboxylates, which were N-alkylated and the resulting secondary amines were cyclised in the presence of a base to give the title compound with 17–92% yield. Alternatively, the amines were first cyclised to 5-unsubstituted pyrazolo[4,3-*c*]pyridine-4-ones. Subsequent N-benzylation afforded three of the title compounds with 36–49% yields. The third method comprises a six-step transformation of methyl acrylate into 1-benzylpiperine-2,4-dione. Treatment of the latter with *N*,*N*-dimethilformamide dimethylacetal (DMFDMA) followed by acid-catalysed cyclisation of the formed enaminone with mthyl-, phenyl- and *tert*-buthylhydrazine afforded the same three title compounds with 79–87% yields. (ŽEROVNIK, Darja, GROŠELJ, Uroš, KRALJ, David, MALAVAŠIČ, Črt, BEZENŠEK, Jure, DAHMAN, Georg, STARE, Katarina, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. *Synthesis* 2010, 3363–3373).

By condensation of malononitrile with dialkyl acetone-1,3-dicarboxylates alkyl (3-cyano-6-alkoxy-2-oxo-1,2-dihydropyridin-4-yl)acetates are formed in contrast to an earlier report according to which diethyl 3-(dicyanomethylene)glutarate was obtained by this reaction. They were transformed with DMFDMA into the corresponding (*E*)-alkyl 2-(3-cyano-6-alkoxy-2-oxo-1,2-dihydropyridin-4-yl)-3-(dimethylamino)propenoates. The structures were confirmed by X-ray structural analysis. (ŠIMUNEK, Petr, BAŠKOVČ, Jernej, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK Branko, *Z. Natforsch*. 2010, 65b, 807–810).

The PF_6 salts of 5-benzyl-1-isopropylidene- and 5-benzyl-1-cinnamylidene-3-methylimidazolidin-4-ones with various substituents in the 2-position have been prepared, and single crystals suitable for X-ray structure determination have been obtained of 14 such compounds. In nine of the structures, the Ph ring of the benzyl group resides above the heterocycle, in contact with the *cis*-substituent at *C*(2) (staggered conformation A); in three structures, the Ph ring lies above the iminium π-plane (staggered conformation B); in two structures, the benzylic C-C bond has an eclipsing conformation which places the Ph ring simultaneously at a maximum distance with its neighbors, the CO group, the N=C-π-system, and the *cis*-substituent at C(2) of the heterocycle. It is suggested by a qualitative conformational analysis that the three staggered conformations of the benzylic C-C bond are all subject to unfavorable steric interactions, so that the eclipsing conformation may be a kind of "*escape*". State-of-the-art quantum-chemical methods, with large AO basic sets (near the limit) for the single-point calculations, were used to compute the structures of seven of the 14 iminium ions, in the two staggered conformations, A and B, with the benzylic Ph group above the ring and above the iminium π-system, respectively. In all cases, the more stable computed conformer ("isolated-molecule" structure) corresponds to the one present in the crystal. The energy differences are small (≤2 kcal/mol) which, together with the result of a potential-curve calculation for the rotation around the benzylic C-C bond of one of the structures suggests that the benzyl group is more or less freely rotating at ambident temperatures. The importance of intramolecular *London* dispersion (benzene ring in contact with the *cis*-substituent in conformation A) for DFT and other quantum-chemical computations is demonstrated; the benzyl-imidazolidinones appear to be ideal systems for detecting dispersion contributions between a benzene ring and alkyl or aryl CH groups. Enylidene ions of the type studied herein are the reactive intermediates of enantioselective organocatalytic conjugate additions, *Diels-Alder* reactions, and many other transformations involving α,β-unsaturated carbonyl compounds. Our experimental and theoretical results are discussed in view of the performance of 5-benzyl-imidazolidinones as enantioselective catalysts. (SEEBACH, Dieter, GROŠELJ, Uroš, SCHWEIZER, W. Bernd, GRIMME, Stefan, MUCK-LICHTENFELD, Christian. *Helvetica Chimica Acta* 2010, *93*, 1).

The structures of iminium salts, formed from diarylprolinol or imidazolidinone derivatives and α,β-unsaturated aldehydes, have been studied by X-ray powder diffraction, single-crystal X-ray analyses, NMR spectroscopy, and DFT calculations. Almost all iminium salts of this type exist in solution as diastereoisomeric mixtures with (*E*)- and (*Z*)-configured +N=C bond geometries. In this study, (*E*)/(*Z*) ratios ranging from 88:12 up to 98:2 and (*E*)/(*Z*) interconversions, were observed. Furthermore, the relative rates, at which the (*E*)- and (Z)-isomers are formed from ammonium salts and α,β-unsaturated aldehydes, were found to differ from the (*E*)/(*Z*) equilibrium ratio in at least two cases; more (*Z*)-isomer is formed kinetically than corresponding to its equilibrium fraction. Given that the enantiomeric product ratios observed in the reactions mediated by organocatalysts of this type are often >=99:1, the (*E*)-iminium-ion intermediates are proposed to react with nucleophiles faster than the (*Z*)-isomers. Possible reasons for higher reactivity of (*E*)-iminium ions and for the kinetic preference of (*Z*)-iminium-ion formation are discussed. The results of related DFT calculations are also reported. (SEEBACH, Dieter, GILMOUR, Ryan, GROŠELJ, Uroš, DENIAU, Gildas, SPARR, Christof, EBERT, Marc-Olivier, BECK, Albert. K, McCUSKER, Lynne B, ŠIŠAK, Dubravka, UCHIMARU, Tadafumi. *Helvetica Chimica Acta* 2010, *93*, 603).

REVIEW ARTICLE

In the review artile entitled **Transformations of Dialkyl Acetone-1,3-dicarboxylates and their (Dimethylamino)methylidene Derivatives** the following transformations are described: Synthesis of 1-substituted 4-ethoxycarbonyl-5-(ethoxycarbonylmethyl)pyrazoles,

pyrazolo[4,3-*c*]pyridine derivatives, pyrazolo[4,3-*d*][1,2]diazepine derivatives, fused pyrazol-3-yl-pyrimidine derivatives and fused pyrazol-3-yl-pyranones, pyrazolo[1,5-*c*]pyrimidin-5-one derivatives, pyridin-4(1*H*)-one derivatives, 4-hydroxypyridin-2(1*H*)-one and pyrano[3,2-*c*]pyridinone derivatives, thiazolo[5,4-*c*]pyridine derivatives, 4-oxo-1,4-dihydropyridazine-3,5-dicarboxylates, heteroaryl substituted pyrimidine derivatives, pyrido[1,2-*a*]pyrimidin-3-yl)thiazole-5-carboxylates and parallel solution-phase synthesis of 1,4-dihydropyridine derivatives. (STANOVNIK, Branko, GROŠELJ, Uroš. *Adv. Heterocycl. Chem.* 2010, *100*, 145–174).

PUBLISHED PLENARY LECTURE

In the plenary lecture entitled **From β-dimethylamino-α-acylamino-α,β-didehydro acid derivatives and related enaminones *via* heterocycles and heterocyclic amino acids to indole alkaloids** we report on the applications of 3-(dimethylamino)propenoates and dimethylaminomethylidene-substitued heterocycles as intermediates for the preparation of various aplysinopsins and their analogues, heteroarylindoles including polycyclic meridianin analogues and analogues with an uracil structural unit, condensed 3-(1*H*-indol-3-yl)-2*H*-pyran-2-ones, and approach towards the preparation of dipodazine analogues and tryprostatin analogues. (STANOVNIK, [Branko. plenary lecture]. V: KARTSEV, Viktor Georgievich (ur.). The Fourth International Conference CBC2010, August 2–6, 2010, Saint-Petersburg. *Sovremenye aspekty himii geterociklov : himija i biologičeskaja aktivnost sintetičeskih i prirodnyh soedinenij*. Moscow: ICSPF (International Charitable Scientific Partnership Foundation), 2010, pp. 161–171.

COOPERATION WITH OTHER UNIVERSITIES AND FOREIGN INSTITUTIONS

Cooperation with Prof. Dr. O. A. Attanasi, University of Urbino (Italia): Reactions of 3-dimethylaminopropenoates and related enaminones with 1,2-diaza-1,3-butadienes (Principal investigator: B.Stanovnik)

Cooperation with Prof. Dr. W. Kantlehner, University of Stuttgart (Germany) in the field of amide acetals and related compound as reagents in organic synthesis (Principal investigator: B. Stanovnik)

Cooperation with Prof. Dr. G. Maas, University of Ulm (Germany) in the field of acetals and related compound as reagents in organic synthesis (Principal investigator B. Stanovnik)

Cooperation in the field of the synthesis of heterocyclic compounds with the Pharmaceutical Company BOEHRINGER-Biberach, Ingelheim (Germany): (Principal investigator: J. Svete)

INTERNATIONAL AWARD

B. Stanovnik was awarded the Gold Badge of International Scientific Partnership Foundation for Contribution to World Science and International Scientific Collaboration (Sankt Peterburg 2010)

OTHER AWARDS

On the ocassion of the 40th Anniversary of the Krka Awards Prof. Stanovnik received an Award for Exceptional Contributions for promoting research among young people

MEMBERSHIP IN INTERNATIONAL SCIENTIFIC COMMITTEES OF INTERNATIONAL CONGRESSES AND SYMPOSIA AND EDITORIAL AND/OR ADVISORY BOARDS OF SCIENTIFIC JOURNALS

B. Stanovnik:

a) Member of the Scientific Committee, European Colloquia of Heterocyclic Chemistry
b) Member of the Scientific Committee, Blue Danube Symposia of Heterocyclic Chemistry
c) Member of the Board of Electronic Journal ARKIVOC, Scientific Editor of ARKIVOC
d) Member of the Advisory Board, Advances in Heterocyclic Chemistry
e) Member of the Scientific Committee, TRAMECH Transmediterranean Symposia on Heterocyclic Chemistry
f) Member of International Advisory Committee of the IBN SINA InternationalConferences on Pure and Applied Heterocyclic Chemistry
g) Member of the Advisory Board, Trends in Heterocyclic Chemistry
h) Head of the Department for international cooperation and coordination of the Slovenian Academy of Sciences and Arts
i) Dean of the class for Natural Sciences at the European Academy of Sciences and Arts, Salzburg, Austria and legat EASA for Slovenia for the period 2010–2014
j) Member of the Advisory Board, Croatica Chemica Acta
k) Member of the Advisory Editorial Board, Journal of Heterocyclic Chemistry
l) 1998–2004 Member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons, Den Haag, The Netherlands

FIZIKALNA KEMIJA
PHYSICAL CHEMISTRY

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0201

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Vojeslav Vlachy

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
prof. dr. Marija Bešter-Rogač
dr. Matjaž Bončina
dr. Jožica Dolenc
dr. Andrej Godec
izr. prof. dr. Barbara Hribar-Lee
izr. prof. dr. Andrej Jamnik
prof. dr. Jože Koller
izr. prof. dr. Ksenija Kogej
izr. prof. dr. Jurij Lah
dr. Miha Lukšič
dr. Črtomir Podlipnik
dr. Iztok Prislan
doc. dr. Jurij Reščič
prof. dr. Jože Škerjanc
dr. Matija Tomšič
doc. dr. Tomaž Urbič
prof. dr. Gorazd Vesnaver
prof. dr. Vojeslav Vlachy

Mladi raziskovalci / Young Researchers
Alan Bizjak
Sašo Čebašek
Igor Drobnak
Ana Kroflič
Andrej Lajovic
Andrej Mernik
Simona Prelesnik

Tehniki / Technicians
Anton Kelbl
Anton Kokalj
Cirila Peklaj

POROČILO O REALIZACIJI PROGRAMA

CILJI IN OSREDNJE TEME PROGRAMA

Raziskave naše skupine prispevajo k razumevanju fizikalnokemijskih procesov, ki se dogajajo v živih bitjih in/ali so pomembni v industriji. Zanimajo nas raztopine in suspenzije nanodelcev, predvsem površinsko aktivnih snovi in polielektrolitov. Nekateri od slednjih so biološko pomembni (proteini in DNK), drugi, to so površinsko aktivne snovi in sintetični polielektroliti, pa se na široko uporabljajo v industriji. Raziskave stabilnosti proteinov in DNK, vezave ligandov na to molekulo in študije podobnosti molekul so pomembne v farmacevtski industriji in bioinženirstvu; prav na teh področjih sodelujemo tudi z industrijo. Merjenja se dopolnjujejo s teoretičnimi raziskavami; namen našega dela je boljše razumevanje procesov na molekularnem nivoju in posredovanje tega znanja študentom ter kolegom v industriji.

ZNANSTVENI DOSEŽKI

1. Nadaljevali smo z raziskavami cikloheksilsulfonske kisline in njenih tetraalkilamonijevih soli [COBISS.SI-ID 34669573, COBISS.SI-ID 33979653] *(FK24, FK13)*, ki lahko služijo kot modelni sistem za študij asociacijskih procesov hidrofobnih ionov v vodnih raztopinah. Asociacijo ionov smo proučevali tudi v razredčenih raztopinah ionskih tekočin 1-butil-3-metilimidazolijevega klorida in tetraflouroborata v metanolu in DMSO. Oba sistema kažeta zmerno asiociacijo v metanolu in bistveno šibkejšo v DMSO [COBISS.SI-ID 33313541] *(FK7)*. Izmerili smo električno prevodnost raztopin metanojske kisline in njenih soli ter ugotovili, da le te v vodi opazno asociirajo [COBISS.SI-ID 33672709] *(FK8)*, najbolj pa je asociacija izražena pri natrijevem formiatu.
2. Pripravili smo vzorce za fazne študije v sistemu polistirensulfonatni anion–kationski surfaktant–voda, določili sestave faz v večfaznih vzorcih ter raziskali njihove strukture z metodo ozkokotnega sipanja svetlobe. Na osnovi dobljenih rezultatov smo napovedali fazno obnašanje na dveh ravninah piramidalnega faznega diagrama.
3. Z reverzno simulacijo Monte Carlo (RMC), ki se uporablja za interpretacijo meritev rentgenskega in nevtronskega sipanja, smo proučevali tekoče alifatske alkohole (metanol, eta-

nol, propanol) [COBISS.SI-ID 34490373] *(FK21)*. Primerjava različnih strategij pri poteku računanja je pokazala, da dobimo najbolj zanesljive napovedi za molekularne modele, če pri postopku RMC eksplicitno upoštevamo vse atome ter vzporedno uporabimo rezultate meritev rentgenskega in nevtronskega sipanja (popolnoma devteriranih vzorcev). Modele, ki jih dobimo z metodo RMC, lahko naknadno izboljšamo še z uporabo rezultatov simulacije molekularne dinamike.

4. Z velekanonično računalniško simulacijo Monte Carlo, s teorijo gostotnega funkcionala ter z integralskimi enačbami smo proučevali strukturne značilnosti modelne tekočine z efektivnim oscilirajočim medmolekulskim potencialom v različnih nehomogenih okoljih [COBISS.SI-ID 34662661] *(FK3)*. Izbrani efektivni potencial je vključeval osnovne prispevke k interakciji med delci mezoskopskih velikosti. Zadovoljivo ujemanje med rezultati simulacij in teorijskimi napovedmi obeta uspešno uporabo teorijskih metod za študij lastnosti kompleksnih tekočin.
5. Razvili smo novo metodo za izračun rentgenskega sipanja modelnih sistemov, ki je osnovana na zapolnitvi manjkajoče okolice vsakega od delcev s povprečno sliko sistema [COBISS.SI-ID 34580741] *(FK11)*. S takšnim pristopom smo uspeli združiti naslednje dobre lastnosti: poljubna skala valovnega vektorja q, zmanjšanje artefaktov zaradi končne velikosti ter veljavnost rezultatov vse do teoretične spodnje meje skale q. Metoda predstavlja precejšnje izboljšanje glede na ostale pristope, ki bodisi žrtvujejo eno od zgoraj navedenih lastnosti bodisi zahtevajo vmesni korak, pri katerem se del razpoložljivih informacij o sistemu izgubi.
6. Z različnimi eksperimentalnimi metodami smo raziskovali hierarhično strukturirane sisteme na osnovi monogliceridov, ki predstavljajo osnovo za vrsto novih materialov, ki obetajo aplikacijo na različnih področjih nanotehnologije ter prehrambne, kozmetične, farmacevtske in kemične industrije. Strnjen pregled te tematike je bil podan v preglednem poglavju v knjižni zbirki »Advances in planar lipid bilayers and liposomes« [COBISS.SI-ID 34569221] *(FK35)*.
7. Izpeljali smo in z metodo integralskih enačb (MSA, HNC) testirali posplošeno Gibbs-Duhemovo enačbo za izračun srednjega aktivnostnega koeficienta elektrolita v prisotnosti poljubne tretje komponente [COBISS.SI-ID 33832197] *(FK6)*. Rezultati nove analitične enačbe se z numeričnimi rezultati na osnovi integralskih enačb odlično ujemajo. V sistemih z veliko zasedenostjo prostora, kjer so tretja komponenta nevtralni delci, smo rezultate za srednji aktivnostni koeficient elektrolita primerjali z rezultati računalniških simulacij [COBISS.SI-ID 34507269] *(FK9)*. Medtem ko MSA, kot tudi modificirana Poisson-Boltzmannova teorija (MPB), dajeta dobre rezultate, so rezultati HNC približka bistveno slabši.
8. Transportne lastnosti kationskih polielektrolitov, ionenov, z različno gostoto naboja in z dvema različnima vrstama protiionov (F^- in Br^-) smo proučevali v članku [COBISS.SI-ID 34322949] *(FK19)*. Iz meritev električne prevodnosti in transportnih števil smo določili delež vezanih protiionov, ki je bil močno odvisen tako od hidrofobnosti polielektrolitske verige kot tudi od vrste protiiona.
9. S pomočjo preprostega dvodimenzionalnega modela vode (MB) smo študirali vpliv tetrametilamonijevega iona (TMA) na topnost hidrofobnega topljenca v odvisnosti od njegove velikosti [COBISS.SI-ID 34600453] *(FK20)*. Rezultati nakazujejo, da tetrametilamonijev ion orientira molekule vode v prvih dveh hidratacijskih lupinah, tako da se mu nepolarni topljenec lahko približa, in s tem pripomore k povečani topnosti hidrofoba.
10. Divodikov trioksid HOOOH je lahko protoniran na terminalnem ali na centralnem kisikovem atomu. V naši raziskavi smo uporabili ab initio metodo CCSD(T) in MP2 z velikim setom baznih funkcij. Zanimala nas je relativna stabilnost obeh možnih oblik protoniranega trioksida. Pokazali smo, da je močno preferirana terminalna oblika, ki ima za 15,8 kcal/mol

nižjo energijo od centralno protonirane oblike. Čeprav obstaja $HOOO(H)H^+$ kot stabilni intermediat, se je pokazalo, da je zelo kratkoživ (aktivacijska energija $E^* = 8{,}6$ kcal/mol) in takoj razpade v H_3O^+ in singletni O_2. Kratkoživost intermediata je verjetno vzrok, da se ga v ^{17}O NMR spektru ni dalo opaziti [COBISS.SI-ID 34295813] *(FK15)*.

11. Za študij lastnosti alkalijskih halogenidov v vodi smo uporabili teorijo na osnovi MSA približka. Molekule vode smo ponazorili kot kroglice s štirimi prostorsko usmerjenimi vezmi, ione pa kot kroglice z »lepljivimi" mesti, kamor se lahko vežejo molekule vode ali drugi ioni. Izbira parametrov je temeljila na dveh predpostavkah: (i) jakost interakcije med enovalentnim ionom in vodo je obratno sorazmerna velikosti iona, in (ii) število kontaktov med vodo in ionom je sorazmerno površini iona. Osmozni koeficienti, ki smo jih izračunali, se zelo dobro ujemajo z eksperimentalnimi (COBISS.SI-ID 34118149) *(FK22)*.
12. V okviru projekta FIRB RETI RBPR05NWWC_04 je dr. Podlipnik od 1. julija do 31. julija 2010 gostoval v skupini profesorja P. Senecija na inštitutu CISI, ki deluje v okviru Milanske univerze. Izsledki raziskav na področju razvoja kinaznih inhibitorjev so objavljeni v članku [COBISS.SI-ID 34621701] *(FK12)*.
13. Delo obravnava termodinamiko interakcije z različnimi alkalijskimi halogenidi v vodi. Prvi smo uspeli ustrezno izmeriti toplotne efekte pri vezanju ionov na lizocim in s pomočjo njihove termodinamske analize razložiti molekularno naravo vezanja. Določili smo konstante vezanja in ugotovili, da sledijo Hofmeistrovi vrsti [COBISS.SI-ID 33831941] *(FK17)*.
14. V nadaljevanju raziskav hidrofobnih kationskih polielektrolitov (ionenov) smo s pomočjo dinamike molekul simulirali raztopine 6,6-ionenov z različnimi protiioni v eksplicitni vodi [COBISS.SI-ID 34400005] *(FK23)*. Rezultate smo tolmačili v luči naših eksperimentalnih rezultatov za te raztopine.
15. Podrobno smo raziskali prednosti in slabosti različnih načinov modelno odvisne termodinamske analize procesov zvitja/razvitja bioloških makromolekul [COBISS.SI-ID 34219269] *(FK18)*. Uspeli smo neposredno povezati termodinamiko zvitja/razvitja toksina CcdB iz bakterije *Vibrio fischeri*, ki povzroča celično smrt bakterij, z njegovimi strukturnimi značilnostmi [COBISS.SI-ID 33885957] *(FK5)*. Na osnovi eksperimentalne in teoretične študije termodinamske stabilnosti različnih mutant modelne dvoverižne DNA smo uspeli določiti in interpretirati različne prisepevke k stabilnosti DNA [COBISS.SI-ID 33744645] *(FK16)*.

DRUGI RELEVANTNI DOSEŽKI

1. Imeli smo več uvodnih predavanj na mednarodnih in domačih konferencah: V. Vlachy, »Polyelectrolytes in water: how the presence of hydrophobic groups modifies the ion-specific effects«, prvo plenarno predavanje na 28th Annual Meeting MLG, September 5–9, 2010, Lviv, Ukrajina; M. Bešter Rogač, »Raztopine elektrolitov – izziv ali zgodovina«, uvodno sekcijsko predavanje, SKD, Maribor, ter univerzah: V. Vlachy, »Ions in water: from Debye--Hückel limiting law to the ion–specific effect«, niz predavanj za podiplomske študente na Kalifornijski univerzi v San Franciscu. Predavanja smo imeli tudi na univerzi v Helsinkih, Karlovi Univerzi v Pragi, na CEA Saclay, Francija, UPMC (Pariz-6) Pariz, Francija.
2. V. Vlachy je v času od 1. 4. 2010 do 1. 5. 2011 gostoval kot »visiting professor« na UPMC (Paris-6), kjer je imel niz predavanj z naslovom »Electrolyte solutions: from Debye–Hückel limiting law to ion–specific effects in presence of hydrophobic groups«.
3. Prof. dr. Andrej Jamnik je dobil Zoisovo priznanje za pomembne dosežke na področju fizikalne kemije.

4. Dr. Andrej Godec je dobil nagrado Maksa Samca (2010) za popularizacijo študijev na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani.
5. Dva člana PS sta bila v tem obdobju na podoktorskem izpopolnjevanju v tujini (dr. Jožica Dolenc – ETH Zürich in dr. Iztok Prislan – ZDA).
6. Sodelovali smo v bilateralnih projektih z Avstrijo, Češko republiko, Poljsko, Madžarsko, Hrvaško, Flandrijo, Portugalsko, ZDA, Finsko in Francijo.
7. Kot partnerji univerze v San Franciscu smo uspeli za nadaljnja štiri leta (2010–2014) pridobiti projekt »Solvation in Biology«, ki ga financira National Institute of Health, ZDA.
8. Sodelovali smo pri dveh COST projektih (D–43 M. Bešter-Rogač in MP–0802 J. Lah).
9. Na obisku smo imeli nekaj uglednih raziskovalcev iz tujine in enega podiplomskega študenta iz Mehike (6 mesecev; mentorica B. Hribar-Lee) ter podiplomsko študentko iz Brna (5 mesecev; mentorica M. Bešter-Rogač).

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

Our research focuses on nanoparticles in solutions and contributes toward better understanding of physico–chemical processes in living beings or/and technologically important processes. Some of them, e.g. proteins and DNA, are of biological importance, while others, e.g. surfactants and synthetic polyelectrolytes, are used in industrial applications. Studies of protein and DNA stability are invaluable for pharmaceutical industry and bioengineering. Wherever possible, the experimental research is complemented with theoretical analysis; the main purpose being to understand these processes on the molecular level and to communicate this knowledge to students and our colleagues in industry.

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

1. Investigation of cyclohexylsulfamic acid [COBISS.SI-ID 34669573] *(FK24)* and its salts has continued with the research on association processes of tetraalkylammonium salts in water solutions [COBISS.SI-ID 33979653] *(FK13)*. It turned out that this system could serve as a model system for study of ion pairing of hydrophobic ions. Further, ion association has been investigated also in diluted solution of ionic liquid 1-buthyl-3-methylimidazolium chlorides and tetrafluoroborate in methanol and DMSO [COBISS.SI-ID 33313541] *(FK7)*. A slight ion association has been observed in both systems, however, essentially weaker in DMSO. The electric conductivity of formic acid and its salts in water has been determined and ion pairing has been studied. Surprisingly, salts show a perceivable ion association which is most expressed in sodium formiate [COBISS.SI-ID 33672709] *(FK8)*.
2. Samples for phase studies in poly(styrenesulfonate anion)-cationic surfactant-water system were prepared, the composition of multiphase samples were analysed and structures of separated phases were determined by small angle X-ray scattering. On the basis of these data phase behaviour was predicted on two planes of the pyramidal phase diagrams.
3. Reverse Monte Carlo (RMC) modeling as a method for the interpretation of experimental X-ray and neutron scattering data was used to study liquid aliphatic alcohols (methanol, ethanol, propanol) [COBISS.SI-ID 34490373] *(FK21)*. By inspecting several computa-

tional strategies it was found out that the most successful strategy towards attaining reliable molecular models, especially if the models were subsequently refined with the results of molecular dynamics simulation can be obtained by parallel application of X-ray and neutron scattering data, the latter being from completely deuterated samples, within an all-atom RMC procedure.

4. Grand canonical Monte Carlo simulation, density functional and integral equation theories were used to study the structure of the model fluid with effective oscillatory interparticle potential in various inhomogeneous environments [COBISS.SI-ID 34662661] *(FK3)*. The chosen effective potential incorporated the basic contributions to the interaction between the particles of mezoscopic dimensions. Satisfactory agreement between the theoretical predictions and the simulation data promises successful application of the pure theories for the investigation of complex fluids.
5. A novel method for calculating X-ray scattering from model systems was developed by complementing the missing surroundings of each particle with an average image of the system [COBISS.SI-ID 34580741] *(FK11)*. The method succeeds in combining several favorable properties: an arbitrary scale of wave vector q, suppression of truncation artifacts and good behavior down to the theoretical lower limit of the q-scale. This represents a significant improvement over other methods which either sacrifice one of the above properties or require an intermediate step in which a part of the available information is lost.
6. Various hierarchically organized systems based on monoglycerides were investigated utilizing different experimental techniques. Deeper understanding of the structure of such systems is crucial for designing new materials applicable in various fields as nanotechnology and food processing, cosmetic, pharmaceutical, and chemical industries. This subject was outlined in an overview chapter in a book series "Advances in planar lipid bilayers and liposomes" [COBISS.SI-ID 34569221] *(FK35)*.
7. An extension of the Gibbs-Duhem equation, appropriate for the calculation of the mean activity coefficient of an electrolyte in the presence of an arbitrary number of cosolute component was tested against the results of the integral equation theories (MSA and HNC) [COBISS.SI-ID 33832197] *(FK6)*. The results of the calculations, utilizing different routes, were in excellent agreement. Activity coefficients for a primitive model electrolyte systems containing a high density neutral component were tested against computer simulations [COBISS.SI-ID 34507269] *(FK9)*. While the MSA, as well as the modified Poisson-Boltzmann theory (MPB), give a good representation of the simulation values in theses systems, the performance of HNC is poorer.
8. The transport properties of cationic polyelectrolytes (ionenes) with different charge density and different kinds of counterions (F^- in Br^-) were studied in [COBISS.SI-ID 34322949] *(FK19)*. Using the electric conductivity and transference number measurements, the fraction of free counterions was estimated and found to be strongly dependent on the hydrophobicity of the polyelectrolyte backbone, as well as of the nature of the counterions.
9. Using a simple two-dimensional water model (MB) the effect of the tetramethylammonium ion (TMA) on the solubility of hydrophobic molecules of diffferent sizes was studied [COBISS.SI-ID 34600453] *(FK20)*. Te results suggest that the water molecules are structured by tetramethylammonium ion in its first two hydration shells, so that the nonpolar solute can actually bind more tightly to the TMA ion than to another hydrophobe, leading to the salting-in effect.
10. Protonated dihydrogen trioxide HOOOH has been postulated in various forms for many years. Protonation can occur at either the terminal $HOOO(H)H^+$ or central $HOOH(OH)^+$

oxygen atom. In the present work we have employed ab initio methods, CCSD(T) and MP2, with a large basis set to determine the relative stability of these species. It is shown that the terminally protonated species is strongly favored relative to the centrally protonated species. Although HOOO(H)H+ exists as a stable intermediate, it is extremely short-lived and rapidly decomposes to H_3O^+ and singlet O_2. Activation energy is 8.6 kcal/mol. The short-lived nature of the intermediate implies that the intermediate species cannot be observed in ^{17}O NMR spectra [COBISS.SI-ID 34295813] *(FK15)*.

11. The solutions of alkali halides in water were studied by the associated MSA theory. Water molecules were modeled as hard spheres with four off-centre sticky sites with capability to bind other waters or ions. The choice of binding parameters was based on two premises: monovalent ion – water interaction is inversely proportional to the Pauling size of the ion and (ii) the number of the ion – water contact is proportional to the surface area of the ion. Osmotic coefficients calculated this way are in very good agreement with the experimental data for alkali halides in water (COBISS.SI-ID 34118149) *(FK22)*.
12. Dr. Podlipnik was a visiting researcher, working in the group of prof. P. Seneci from the Institute CISI (University of Milano) from July 1st to July 31st 2010. He was engaged in the FIRB RETI RBPR05NWWC_04 project. Their joint contribution in the field of design of kinase inhibitors was published in the article [COBISS.SI-ID 34621701] *(FK12)*.
13. We studied the thermodynamics of lysozyme with various alkali halide salts interactions in water. For the first time we have been able to measure the heat effects of ion-binding to the lysozyme molecule and by thermodynamic analysis we explained the molecular nature of this binding. We determined the binding constant and proved that they follow the Hofmeister series [COBISS.SI-ID 33831941] *(FK17)*.
14. In continuation of our study of hydrophobic polyelectrolytes (ionenes) we presented molecular dynamics simulation of 6,6-ionenes with various counterions in explicit water [COBISS.SI-ID 34400005] *(FK23)*. The results were explained in view of the experimental data for this system.
15. We have performed a detailed study of advantages and disadvantages of various types of model-based thermodynamic analyses of biomolecular folding/unfolding processes [COBISS.SI-ID 34219269] *(FK18)*. We have successfully correlated thermodynamics of folding/unfolding of the toxin CcdB, the gyrase poison from bacteria *Vibrio fischeri*, to its structural features [COBISS.SI-ID 33885957] *(FK5)*. Based on the experimental data and theoretical study of thermodynamic stability of a model DNA duplex and some of its mutants we were able to determine and interpret various contributions to the DNA stability [COBISS.SI-ID 33744645] *(FK16)*.

OTHER RELEVANT ACHIEVEMENTS

1. Our group delivered several plenary or keynote lectures at domestic and international scientific conferences: V. Vlachy, “Polyelectrolytes in water: how the presence of hydrophobic groups modifies the ion–specific effects”, introductory plenary lecture at the 28th Annual Meeting MLG, September 5–9, 2010, Lviv, Ukraine; M. Bešter Rogač, “Electrolyte solutions – challenge or history”, keynote lecture at SKD, Maribor) and Universities: V. Vlachy, “Ions in water: from Debye–Hückel limiting law to the ion–specific effect”, set of lectures for graduate students at the UC San Francisco. Other lectures were given at the University in Helsinki, Charles University Prague, CEA Saclay, France, U. Pierre and M. Curie, Paris, France, and other institutions.

2. From April 1, 2010 to May 1, 2011 V. Vlachy served as a “visiting professor” at U. Pierre and Marie Curie (Paris-6), where he delivered a set of lectures entitled: “Electrolyte solutions: from Debye–Hückel limiting law to ion–specific effects in the presence of hydrophobic groups”.
3. Prof. Dr. Andrej Jamnik has been awarded the “Zois Award” for significant contributions to science in the field of Physical Chemistry.
4. Dr. Andrej Godec was the receiver of the Maks Samec Award (2010) awarded by the Faculty of chemistry and chemical technology, University of Ljubljana for the popularization of chemical studies.
5. Two members of the group were on longer postdoctoral visiting programmes at foreign universities (Dr. Jožica Dolenc – ETH Zürich and Dr. Iztok Prislan – USA).
6. We have established formal bilateral collaboration with researchers in Austria, Czech Republic, Poland, Hungary, Croatia, Flanders, Portugal, USA, Finland, and France.
7. As partners of the UC San Francisco, we managed to obtain financial support from the National Institute of Health, USA, to work on the project “Solvation in Biology” for the next four years (2010–2014).
8. We participated in two COST projects (D–43 M. Bešter-Rogač and MP–0802 J. Lah).
9. We have hosted several distiguished foreign researchers and one postgraduate student (6 months; mentor B. Hribar-Lee) from Mexico and a postgraduate student from Brno (5 months; mentor M. Bešter-Rogač).

ORGANSKA KEMIJA: SINTEZA, STRUKTURA IN APLIKACIJA
ORGANIC CHEMISTRY: SYNTHESIS, STRUCTURE, AND APPLICATION

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0230

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Marijan Kočevar

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
prof. dr. Slovenko Polanc
prof. dr. Marijan Kočevar
prof. dr. Andrej Petrič
izr. prof. dr. Bojan Verček
izr. prof. dr. Janez Košmrlj
doc. dr. Bogdan Štefane
doc. dr. Franc Požgan
dr. Krištof Kranjc, znan. sod.
dr. Damijana Urankar
Nenad Maraš, univ. dipl. kem.

Mladi raziskovalci / Young Researchers
Bojan Burja
Jure Hren
Vita Majce
Amadej Juranovič
Martin Gazvoda
Marko Krivec

Tehniki / Technicians
Zdenka Kadunc
Irena Povalej

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Cilj raziskovalnega programa je razvijanje sintez spojin z visoko atomsko ekonomičnostjo za znanstvene in aplikativne namene pod okolju prijaznimi pogoji. Zastavljene cilje dosegamo z lastnim kreativnim delom, s povezavo z več mednarodnimi raziskovalnimi skupinami ter v sodelovanju z domačimi akademskimi skupinami in industrijo. V letu 2010 je bilo naše raziskovalno delo usmerjeno v načrtovanje novih sinteznih metod, reagentov in reakcij, ki bi omogočile sintezo spojin s ciljnimi biološkimi aktivnostmi.

OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

V sodelovanju s francoskimi raziskovalci smo študirali direktno ariliranje heteroaromatov (furan, tiofen, izoksazol, tiazol) substituiranih s prosto hidroksialkilno skupino. Uporabljali smo nizke koncentracije $Pd(OAc)_2$ (0.01–0.5 mol %) kot predkatalizatorja, brez dodatka liganda in brez zaščite/odščite funkcionalne skupine. Reakcija je potekla preko aktivacije C–H vezi na heteroaromatu, nadaljnja funkcionalizacija s (hetero)aril bromidi pa je selektivno vodila do nastanka 5-ariliranih produktov. V primerjavi s klasičnimi reakcijami pripajanja predstavlja naša metodologija ekološko in ekonomsko učinkovitejši pristop do tovrstnih produktov (ROGER, Julien, POŽGAN, Franc, DOUCET, Henri, *Adv. Synth. Catal.* 2010, *352*, 696).

Na področju zelene kemije smo objavili pregledni članek o organski sintezi pod vplivom mikrovalov. Poudarek je bil na novejših rezultatih na tem področju, vključujoč tudi naše transformacije pod mikrovalovnimi pogoji (KRANJC, Krištof, KOČEVAR, Marijan, *Curr. Org. Chem.* 2010, *14*, 1050). Na področju nenasičenih heterocikličnih aminokislinskih derivatov smo izvedli eksperimentalno študijo, z vključeno kinetično analizo in DFT računalniško obdelavo Diels−Alderjeve reakcije cikloadicije 2*H*-piran-2-onov in različnih alkinov. Posebno pozornost smo namenili *N*,*N*-dietilpropinaminu kot dienofilu. Dokazali smo, da takšne pretvorbe potekajo preko zelo polarnih prehodnih stanj. Naj še omenimo, da relativno velik prenos naboja in velika nesimetrija pri tvorbi vezi C–C pri reakciji 2*H*-piran-2-onskega derivata z *N*,*N*-dietilpropinaminom mogoče podpira celo ionski (»zwitterionski«) značaj teh reakcij (ŠTEFANE, Bogdan, PERDIH, Andrej, PEVEC, Andrej, ŠOLMAJER, Tomaž, KOČEVAR, Marijan, *Eur. J. Org. Chem.* 2010, 5870).

Na področju borovih kelatov smo raziskali kemoselektivne adicije organolitijevih reagentov na BF_2-kelate β-ketoestrov kjer nastanejo ustrezni 1,3-dioksa-BF_2 kompleksi, katerim smo v nadaljevanju ovrednotili njihove fluorescenčne lastnosti (ŠTEFANE, Bogdan, *Org. Lett.* 2010, *12*, 2900). V okviru sodelovanja s Fakulteto za farmacijo smo sintetizirali in raziskali inhibitorne lastnosti različnih 1,3,5-triazin-2(1*H*)-onov na MurF encim. V okviru teh raziskav so bile izvedene tudi študije molekularnega sidranja najperspektivnejše spojine v aktivno mesto MurF encima (SOSIČ, Izidor, ŠTEFANE, Bogdan, KOVAČ, Andreja, TURK, Samo, BLANOT, Didier, GOBEC, Stanislav, *Heterocycles* 2010, *81*, 91). B. Štefane je v okviru gostova-

nja na University of Maryland, ZDA, raziskoval nove sintezne poti Rh-kataliziranih intramolekularnih C–H vrivanj diazospojin (WANG, Jingxin, ŠTEFANE, Bogdan, JABER, Deana, SMITH, Jacqueline A. I., VICKERY, Christopher, DIOP, Mouhamed, SINTIM, Herman O. *Angew. Chem. (Int. ed., Print)* 2010, *4*9, 3964).

Pokazali smo, da lahko α,β-didehidro-α-aminokislinske (DDAA) derivate, ki imajo na β-mestu pirazolski ali izoksazolski obroč, z uporabo diazometana uspešno pretvorimo v ustrezne metilne estre. Z uporabo te metode C=C dvojna vez DDAA derivatov z diazometanom ne reagira, ampak se selektivno metilira samo karboksilna skupina (POŽGAN, Franc, LUKMAN, Klavdija, KOČEVAR, Marijan, *Heterocycles* 2010, *82*, 543).

Z rentgensko difrakcijsko analizo je bila potrjena struktura 3-benzamido-1-benzoil-1*H*-pirol--2(5*H*)-ona, spojine, ki nastane pri segrevanju 2-benzoilamino-3-kloropropenojske kisline v piridinu (KASUNIČ, Marta, VERČEK, Bojan, MUŠIČ, Irena, GOLOBIČ, Amalija, *Acta Crystallographica. E, Structure Reports* 2010, *E66*, o687).

S kvaternimi amonijevimi solmi smo izvedli alkiliranje fenolov in pri tem dobili serijo alkil aril etrov. Reakcija je bila uspešno izvedena v polietilenglikolu (PEG) pri temperaturah 150–160 °C in v prisotnosti K_2CO_3 ali NaOH kot baze (MARAŠ, Nenad, POLANC, Slovenko, KOČEVAR, Marijan, *Acta Chim. Slov*. 2010, *57*, 29).

V sodelovanju s partnerji iz farmacevtske industrije Lek smo prvi razvili način za sintezo statinov preko laktonskega intermediata. Kemijo smo prikazali na primeru sinteze rosuvastatina. Ključna stopnja je zelo selektivna Wittigova olefinacija med primernim heterocikličnim ilidom in β-TBSO funkcionaliziranim δ-formil-δ-valerolaktonom v 4-*O*-TBS-zaščiten statinski lakton. Wittigovo reakcijo, odstranitev zaščite, hidrolizo laktona in izmenjavo kationa v rosuvastatin kalcij smo izvedli kot »one-pot« reakcijo z odličnim celokupnim izkoristkom in brez opazne epimerizacije. Ta nov konvergenten pristop, ki ga odlikuje še dejstvo, da ne zahteva kriogenih reakcijskih pogojev, je boljši od vseh do sedaj opisanih načinov za pripravo rosuvastatina (ČASAR, Zdenko, STEINBÜCHER, Miha, KOŠMRLJ, Janez, *J. Org. Chem.* 2010, *75*, 6681). Ta članek je bil uvrščen med 20 najbolj branih člankov v reviji *The Journal of Organic Chemistry* v oktobru 2010 in je omenjen v »Highlights from the Literature« v *Organic Process Research & Development* 2010, *14*, 1276. Za pripravo ključnega heterocikličnega intermediata, za sintezo rosuvastatina po zgoraj opisani metodi, smo vložili patentno prijavo.

Sintetizirali smo serijo kombretastatinov s prikondenziranim pirazolonskim obročem in ugotavljali njihovo citotoksičnost ter antitubulinsko aktivnost. Eden od hidrazidov, namreč prekurzor kombretastatina s prikondenziranim pirazolonskim obročem, ki je imel 2-naftilno skupino, kot tudi trije kombretastatini s prikondenziranim pirazolonskim obročem, so bili zelo citotoksični na različne tumorske celice, vključno s tistimi, ki so rezistentne na cisplatin. Iste spojine so bile tudi najboljši inhibitorji polimerizacije tubulina. Rezultati molekularnega modeliranja so pokazali, da se te spojine vežejo na kolhicinsko vezavno mesto tubulinskega heterodimera. Že omenjeni hidrazid blokira HeLa celice v G2/M fazi celičnega cikla in močno vpliva na obliko celice in mikrotubulinsko mrežo (BURJA, Bojan, ČIMBORA, Tamara, TOMIĆ, Sanja, JELUŠIĆ, Tihana, KOČEVAR, Marijan, POLANC, Slovenko, OSMAK, Maja, *Bioorg. Med. Chem.* 2010, *18*, 2375).

V sodelovanju med raziskovalnimi skupinami z University of California at Los Angeles, Indiana University ter Medicinske fakultete Univerze v Ljubljani smo raziskali možnost razširitve uporabe [^{18}F]-FDDNP PET na področje diagnostike, ne samo Alzheimerjeve, ampak tudi drugih nevrodegenerativnih bolezni, za katere je tudi značilno izločanje proteinskih agregatov v možganskem tkivu. Takšna patologija je značilna tudi za bolnike z redko Gerstmann-Sträus-

sler-Scheinkerjevo boleznijo. Objavili smo rezultate primerjave detekcije proteinskih agregatov *in vitro* in *in vivo* z [^{18}F]-FDDNP PET ter [^{18}F]-FDG PET in slikanjem z magnetno resonanco (MRI). Ugotovili smo, da sintetizirana spojina [^{18}F]-FDDNP omogoča uspešno detekcijo prionskih proteinskih agregatov s pozitronsko emisijsko tomografijo (PET) v možganih oseb z dedno PRNP mutacijo in omogoča časovno zasledovanje napredovanja bolezni in uspešnost terapevtskih posegov (KEPE, Vladimir, GHETTI, Bernardino, FARLOW, Martin R., BRESJANAC, Mara, MILLER, Karen, HUANG, Sung-Cheng, WONG, Koon-Pong, MURRELL, Jill Renee, PICCARDO, Pedro, EPPERSON, Francine, REPOVŠ, Grega, ŠMID, Lojze, PETRIČ, Andrej, SIDDARTH, Prabha, LIU, Jie, SATYAMURTHY, Nagichettiar, SMALL, Gary W., BARRIO, Jorge R. *Brain Pathol*. 2010, *20*, 419).

Propargil substituirane diazene, ki smo jih pripravili po dveh različnih poteh, smo študirali kot alkinske klik komponente v azid-alkin cikloadicijah, kataliziranih z bakrom(I). Za azidne komponente smo izbrali 2-(azidometil)piridin in štiri α-azido-ω-aminoalkane (C2 do C5). Medtem, ko so reakcije z α-azido-ω-aminoalkani v prisotnosti bakrovega(II) sulfata in brez dodanega reducenta potekle v nekaj minutah, so reakcije z 2-(azidometil)piridinom potekale veliko počasneje (2–24 ur), kljub dodatku kovinskega bakra v reakcijsko zmes. To razliko v reaktivnosti smo študirali in predpostavili verjetni mehanizem (URANKAR, Damijana, STEINBÜCHER, Miha, KOSJEK, Jaka, KOŠMRLJ, Janez, *Tetrahedron* 2010, *66*, 2602).

Razvili smo alternativen, blag in zelo učinkovit pristop za pripravo kompleksov platine z bioaktivnimi ligandi. Osnovna ideja je selektivna, z bakrom-katalizirana 1,3-dipolarna cikloadicija med terminalnim alkinom in azidom, ki je že del kompleksa platine. Pristop, ki smo ga prikazali pri pripravi novih diazenkarboksamid-karboplatin analogov, je boljši od dosedanjih sinteznih poti (URANKAR, Damijana, KOŠMRLJ, Janez, *Inorg. Chim. Acta*. 2010, *363*, 3817).

Eksperimentalno in teoretično smo pokazali kako lahko dušikov N2 atom 1,2,3-triazola (»klik triazola«) aktivno sodeluje v koordinaciji na različne ione kovin prehoda, kot so Pt(II), Pd(II), Cu(II), Ru(II), Ag(I). Pripravili smo modelno spojino 4-fenil-1-(2-pikolil)-1*H*-1,2,3-triazol (**L**) in njeno koordinacijo na kovinske ione študirali s *cis*-[$PtCl_2(DMSO)_2$], [$Pd(CH_3CN)_4$]$(BF_4)_2$, $CuCl_2$, [$RuCl(\mu\text{-}Cl)(\eta^6\text{-}p\text{-cimen})]_2$ in $AgNO_3$. Nastali so stabilni kelati [$PtCl_2$**L**], [Pd(**L**)$_2$]$(BF_4)_2$, [$CuCl_2$(**L**)$_2$], [$RuCl(\eta^6\text{-}p\text{-cimen})$**L**]OTf in [$Ag_2$(**L**)$_2(NO_3)_2$] s 60–98 % izkoristki. Strukture kompleksov smo nedvoumno potrdili z NMR spektroskopijo in rentgensko difrakcijsko analizo. Naše teoretične študije kažejo, da je stabilizacija nastalih koordinacijskih spojin možna predvsem zaradi učinkovite delokalizacije elektronov s kovine v π-razvezno orbitalo aromatskega liganda in ne toliko zaradi elektrostatskih interakcij, kar je pred tem navajala literatura (URANKAR, Damijana, PINTER, Balazs, PEVEC, Andrej, DE PROFT, Frank, TUREL, Iztok, KOŠMRLJ, Janez, *Inorg. Chem.* 2010, *49*, 4820).

Ugotovili smo, da je 1-pikolil-1,2,3-triazol vsestransko uporaben ligand, ki se na ione kovin, kot so rodij, zlato, paladij in živo srebro, lahko veže na eno-, dvo- in večvezen način. To smo pokazali na modelni spojini 4-fenil-1-(2-pikolil)-1*H*-1,2,3-triazolu (**L**) in njegovih kompleksih: [$Rh_2(O_2CCH_3)_4$(**L**)$_2$], [$PdCl_3$(H**L**)]·H_2O, (H**L**)$_2$[$AuCl_4$]Cl in [Hg_4Br_8(**L**)$_2]_n$. Strukture spojin smo potrdili z rentgensko difrakcijsko analizo. V rodijevem kompleksu je ligand **L** aksialno koordiniran s piridinskim N4 atomom. V paladijevi spojini je N4 protoniran ligand **L** (H**L**$^+$) koordiniran s triazolnim N3 atomom. Ionski kompleks z zlatom je sestavljen iz treh tipov ionov: H**L**$^+$, $AuCl_4^-$ in Cl^-, ki so med seboj povezani z vodikovimi vezmi. Živosrebrova spojina je koordinacijski polimer, v katerem po dva liganda **L** stabilizirata Hg_4Br_8 verigo, v koordinaciji pa sodelujejo piridinski N4 atom in triazolna dušikova atoma N2 ter N3. Pokazali smo, da ta ligand v koordinacijskih spojinah omogoča najrazličnejše supramo-

lekularne povezave, od vodikovih vezi, C–H•••π in π–π interakcij (URANKAR, Damijana, PEVEC, Andrej, TUREL, Iztok, KOŠMRLJ, Janez, *Cryst. Growth Des.* 2010, *10*, 4920). Ta članek je bil uvrščen med 20 najbolj branih člankov v reviji *Crystal Growth & Design* v novembru 2010.

Naredili smo primerjalno študijo selektivnega glukoziliranja *N*-substituiranih 4-hidroksikinolin-2(1*H*)-onov v 4-(tetra-*O*-acetil-β-D-glukopiranoziloksi)kinolin-2(1*H*)-one. Testirali smo štiri glikozil-donorje in različne reakcijske pogoje. Najboljše rezultate smo dobili s tetra-*O*-acetil-*α*-D-glukopiranozil bromidom v CH_3CN in v kombinaciji s Cs_2CO_3. V nekaterih primerih je poleg 4-*O*-glukoziliranja poteklo še 2-*O*-glukoziliranje, pri čemer so nastali ustrezni 2,4-bis(tetra-*O*-acetil-β-D-glukopiranoziloksi)kinolini. Med odstranitvijo acetilnih skupin s Et_3N v MeOH v ustrezne 4-(β-D-glukopiranoziloksi)kinolin-2(1*H*)-one smo v nekaterih primerih opazili cepitev vezi sladkor–aglikon (KIMMEL, Roman, KAFKA, Stanislav, KOŠMRLJ, Janez, *Carbohydr. Res.* 2010, *345*, 768). Strukturo enega od zgoraj navedenih produktov smo študirali z rentgensko difrakcijsko analizo (KIMMEL, Roman, NEČAS, Marek, KAFKA, Stanislav, KOŠMRLJ, Janez, VÍCHA, Robert, *Acta Crystallographica. E, Structure Reports* 2010, *E66*, o1328).

Naše raziskave so prispevale nova znanja na področju sinteze kompleksnih spojin, od sinteze novih tipov gradnikov do razvoja novih sinteznih metod. Nove reakcije organske sinteze smo temeljito raziskali in razložili. Po drugi strani pa smo sintetizirali tudi nekaj novih biološko aktivnih spojin. Nekatere spojine, ki smo jih pripravili, so se izkazale kot primerne za diagnosticiranje določenih bolezenskih stanj.

DRUGI RELEVANTNI DOSEŽKI

MEDNARODNI PATENT

– ANDERS, Manfred, LICHTBLAU, Dirk Andreas, KOLAR, Jana, MALEŠIČ, Jasna, STRLIČ, Matija, ŠALA, Martin, KOČEVAR, Marijan. *Antioxidant for an organic material and method for treating the same : patent : EP 1664431 (B1), 2010-08-04*. [S. l.]: European Patent Office, 2010. 21 str., ilustr.

  Pri naših raziskavah v 5. okvirnem programu (FP project InkCor, EVKA4-CT-2001-00049, koordinatorica J. Kolar) nas je zanimala inhibicija propadanja galnih črnil zaradi prisotnosti železovih ionov. Vložili smo mednarodno patentno prijavo (2005); leta 2010 pa je bil za prijavo dodeljen EU patent. Pripravili smo dve ciljni spojini (mio-inozitol fosfata) in za obe dokazali, da na podobnem nivoju kot dodekanatrijeva sol fitinske kisline preprečujeta propadanje galnih črnil ob prisotnosti železa v različnih celuloznih vzorcih. Zaradi tega sta spojini uporabni za zaščito papirnih dokumentov.

PATENTNE PRIJAVE

1. OSMAK, Maja, POLANC, Slovenko, ČIMBORA, Tamara, BROZOVIĆ, A., KOČEVAR, Marijan, MAJCE, Vita, ALIČ, Branko. *Analogues of 1,3-bis(4-nitrophenyl)triazenes, their pharmaceutically acceptable salts and N-acyl derivatives for tumor treatment : patentna prijava : WO 2010103338 (A1), 2010-09-16*. [S. l.]: World Intellectual Property Organization, 2010. 21 str., ilustr.

   Zdravljenje raka zahteva vedno nova in učinkovitejša zdravila, ki bi izboljšala uspeh kemoterapije. Naša patentna prijava obravnava analoge 1,3-bis(4-nitrofenil)triazenov, njihove

farmacevtsko sprejemljive soli in *N*-acil derivate kot obetajoče kandidate za razvoj novih zdravil za zdravljenje pacientov, obolelih za rakom. Navedene spojine so citotoksične pri zelo nizkih koncentracijah (IC50 0,22 do 12,8 μM) in so dobro topne. Naše raziskave kažejo, da bi lahko uporabili zgoraj omenjene spojine za zdravljenje raka bodisi same, ali pa v kombinaciji z drugimi zdravili.

2. ČASAR, Zdenko, KOŠMRLJ, Janez. *Key intermediates for the synthesis of rosuvastatin or pharmaceutically acceptable salts thereof : international application no.: WO 2010/086438 A1*. [S. l.]: World Intellectual Property Organization, International Bureau, 5.08.2010. 40 str.

   Ta patentna prijava je povezana s pripravo *N*-(4-(4-fluorofenil)-6-izopropil-5-metilpirimidin-2-il)-*N*-metilmetansulfonamida, *N*-(5-(bromometil)-4-(4-fluorofenil)-6-izopropilpirimidin-2-il)-*N*-metilmetansulfonamida in *N*-(4-(4-fluorofenil)-5-(hidroksmetil)-6-izopropilpirimidin-2-il)-*N*-metilmetansulfonamida, treh ključnih intermediatov za pripravo rosuvastatina.

3. KIDEMET, Davor, ZUPET, Rok, SMODIŠ, Janez, ŠTEFANE, Bogdan, POŽGAN, Franc. *Process and intermediates for the preparation of aliskiren: Application No. 09176568.5-1211*. Rijswijk: European Patent Office, 11. 1. 2010.
4. TUREL, Iztok, KLJUN, Jakob, ŠTEFANE, Bogdan. *Postopek za pripravo racemnega nikotina : št. P-201000450*. Ljubljana: Urad Republike Slovenije za intelekturalno lastnino, 22. 12. 2010. 7 str.

MEDNARODNA NAGRADA

Doc. dr. Bogdan Štefane je bil nagrajen s prestižno Fulbrightovo štipendijo v okviru katere je od oktobra 2009 do marca 2010 gostoval na University of Maryland, ZDA, kjer je v okviru postdoktorskega izpopolnjevanja sodeloval pri raziskavah signalnih poti bakterijske virulence. Njegove raziskave so bile objavljene v dveh izjemnih znanstvenih publikacijah (ena v 2011):

1. WANG, Jingxin, ŠTEFANE, Bogdan, JABER, Deana, SMITH, Jacqueline A. I., VICKERY, Christopher, DIOP, Mouhamed, SINTIM, Herman O. Remote C-H functionalization: using the N-O moiety as a atom-economical tether to obtain 1,5- and the rare 1,7-C-H insertions. *Angew. Chem. (Int. ed., Print)* 2010, *49*, 3964.
2. NAKAYAMA, Shizuka, KELSEY, Ilana, WANG, Jingxin, ROELOFS, Kevin, ŠTEFANE, Bogdan, LUO, Yiling, LEE, Vincent T., SINTIM, Herman O. Thiazole orange-induced c--di-GMP quadruplex formation facilitates a simple fluorescent detection of this ubiquitous biofilm regulating molecule. *J. Am. Chem. Soc.* 2011, *133*, 4856.

PLENARNA IN VABLJENA PREDAVANJA

Člani programske skupine so bili avtorji več plenarnih in vabljenih predavanj na mednarodnih konferencah oz. domači konferenci.

DRUGE DEJAVNOSTI IN PRIZNANJA

M. Kočevar je član upravnega odbora COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011).

Na povabilo predsednika IUPAC Professor Jun-Il Jina je M. Kočevar z letom 2010 postal IUPAC Fellow (Glej: http://www.iupac.org/web/per/kocevar).

Uredniško delo: K. Kranjc je član uredniškega sveta *Acta Chimica Slovenica* (ACSi), (2007−), M. Kočevar član uredniškega odbora *Periodica Polytechnica. Chemical Engineering* (2003−), S. Polanc pa član uredniškega odbora *Topics in Heterocyclic Chemistry* (2008−).

Člani programske skupine Andrej Petrič, Bogdan Štefane in Franc Požgan z delom raziskovalnih aktivnosti sodelujejo v EN-FIST centru odličnosti (CO EN-FIST; http://enfist.si/). V sklopu raziskovalno-razvojnega projekta RRP11: »Spojine za diagnostiko in terapijo v medicini« poskušajo z uvajanjem sodobnih sinteznih pristopov, kot so metateza in cross-coupling reakcije, izboljšati učinkovitost sinteze znanih farmacevtskih učinkovin in molekularnih sond za diagnostiko v medicini, kakor tudi pripraviti nove spojine.

Član programske skupine Andrej Petrič je predstojnik Centra za NMR spektroskopijo na UL FKKT (http://nmr-slave.fkkt.uni-lj.si). Skupaj s članom programske skupine Janezom Košmrljem sta, poleg skrbi za redno uporabo in vzdrževanje obstoječega, 15 let starega 300 MHz NMR inštrumenta, izpeljala nabavo in inštalacijo dveh novih NMR inštrumentov, katerih sofinanciranje je ARRS odobrila na osnovi razpisa za nakup opreme v sklopu 14. paketa. En inštrument deluje v laboratoriju na FKKT, drugi pa v laboratoriju FFA. Oba nova inštrumenta sta v redni uporabi od decembra 2010. Rezultati raziskav v letu 2010, pri katerih so raziskovalci s FKKT in FFA uporabljali meritve z opremo NMR centra, so bili objavljeni v 60 izvirnih in preglednih znanstvenih člankih, desetih vabljenih predavanjih, 89 prispevkih na konferencah ter 5 patentnih prijavah in 1 patentu. Oprema infrastrukturnega centra je bila uporabljena tudi pri raziskavah v sklopu 8 doktorskih disertacij ter dveh magistrskih in 28 diplomskih del.

Člana programske skupine Janez Košmrlj in Andrej Petrič sta izpeljala nabavo in inštalacijo novega Agilent 6224 Accurate Mass TOF LC/MS inštrumenta. Inštrument je bil financiran s strani FKKT in bo v okviru infrastrukturnega centra v uporabi z januarjem 2011.

Člani programske skupine smo sodelovali v bilateralnih projektih z Argentino, Hrvaško, Češko republiko in Romunijo ter vodili več industrijskih in drugih projektov.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

The goal of our research programme is focused on the development of syntheses of target molecules for scientific purposes and their applications, with emphasis on eco-friendly conditions and high atom economy. We are pursuing these goals by creative work, through cooperation in various international programmes, as well as with research programmes in several academic institutions in Slovenia and the industry. Our research efforts in 2010 were directed into developing new synthetic methods, reagents, and reactions to provide access to the compounds possessing target biological activities.

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

In collaboration with French researchers we studied direct arylation of heteroaromatics (furan, thiophene, isoxazole, thiazole) bearing unprotected hydroxyalkyl group by using ligand-free low-loading $Pd(OAc)_2$ (0.01–0.5 mol%) as the precatalyst without any protection/deprotection sequence of functional groups. The reaction proceeded *via* activation of C–H bond of

the heteroaromatic compound, which was further functionalized with (hetero)aryl bromides, thus selectively leading to 5-arylated products. Compared with classical cross-coupling reactions our methodology represents a more environmentally and economically attractive access to such arylated products (ROGER, Julien, POŽGAN, Franc, DOUCET, Henri, *Adv. Synth. Catal.* 2010, *352*, 696).

Within the framework of green chemistry we have published a review about microwave-assisted organic synthesis, with the emphasis on recent results in this field, including our microwave-assisted transformations (KRANJC, Krištof, KOČEVAR, Marijan, *Curr. Org. Chem.* 2010, *14*, 1050). In the field of unsaturated heterocyclic amino acid derivatives we performed an experimental study, also including a kinetic analysis, and a DFT computational study of the Diels−Alder cycloaddition reaction of 2*H*-pyran-2-ones with alkynes. A special attention was given to *N*,*N*-diethylpropyneamine as a dienophil. We have shown that such transformations take place via highly polar transition state. We would also like to note that a relatively large charge transfer and high non-symmetry of the C–C bond formation in the reaction of a 2*H*-pyran-2-one derivative with *N*,*N*-diethylpropyneamine might even support the ionic (zwitterionic) character of these reactions (ŠTEFANE, Bogdan, PERDIH, Andrej, PEVEC, Andrej, ŠOLMAJER, Tomaž, KOČEVAR, Marijan, *Eur. J. Org. Chem.* 2010, 5870).

Additionally, we have investigated a short, mild and chemoselective addition of organolithium reagents to BF_2 complexes of β-ketoesters yielding the corresponding 1,3-dioxa-BF_2 complexes. The latter can be easily transformed to different 1,3-diketones. In general, the method allows for direct transformation of 3-oxopropenoates into 1,3-diketones which have, as a starting material, great synthetic value in organic synthesis. In addition, the fluorescent properties of 1,3-dioxa-BF_2 chelates were investigated (ŠTEFANE, Bogdan, *Org. Lett.* 2010, *12*, 2900). In collaboration with the Faculty of Pharmacy we have synthesized and evaluated inhibitory activities of various 2,4,6-trisubstituted 1,3,5-triazines on MurF enzyme. Additionally, to locate the possible binding orientation of the most potent compound with the active site of MurF enzyme, a docking experiment was performed (SOSIČ, Izidor, ŠTEFANE, Bogdan, KOVAČ, Andreja, TURK, Samo, BLANOT, Didier, GOBEC, Stanislav, *Heterocycles* 2010, *81*, 91). As a visiting scholar at the University of Maryland, USA, B. Štefane was investigating new reaction pathways of rhodium-catalyzed intramolecular C–H insertions with diazo compounds (WANG, Jingxin, ŠTEFANE, Bogdan, JABER, Deana, SMITH, Jacqueline A. I., VICKERY, Christopher, DIOP, Mouhamed, SINTIM, Herman O. *Angew. Chem. (Int. ed., Print)* 2010, *49*, 3964).

We have shown that α,β-didehydro-α-amino acid (DDAA) derivatives containing a pyrazole or an isoxazole ring at the β-position can be successfully transformed with diazomethane into the corresponding methyl esters. With this method, the double C=C bond of the DDAA derivatives was not affected, thus selectively giving the corresponding esters (POŽGAN, Franc, LUKMAN, Klavdija, KOČEVAR, Marijan, *Heterocycles* 2010, *82*, 543).

The structure of 3-benzamido-1-benzoyl-1*H*-pyrrol-2(5*H*)-one, a compound which is formed by heating 2-benzoylamino-3-chloropropenoic acid in pyridine, was confirmed by single crystal X-ray diffraction analysis (KASUNIČ, Marta, VERČEK, Bojan, MUŠIČ, Irena, GOLOBIČ, Amalija, *Acta Crystallographica. E, Structure Reports* 2010, *E66*, o687).

Alkylation of phenols was performed with quaternary ammonium salts, yielding a series of alkyl aryl ethers. The reaction was efficiently carried out in polyethyleneglycol (PEG) at temperatures 150–160 °C and in the presence of either K_2CO_3 or NaOH as a base (MARAŠ, Nenad, POLANC, Slovenko, KOČEVAR, Marijan, *Acta Chim. Slov*. 2010, *57*, 29).

In collaboration with Lek Pharmaceuticals, we have developed the first entry into statins via a lactone intermediate. The chemistry is demonstrated by the preparation of rosuvastatin. The key step of this approach is a highly selective Wittig olefination between the appropriate heterocyclic ylide and β-TBSO functionalized δ-formyl-δ-valerolactone into 4-*O*-TBS-protected statin lactone. Following Wittig coupling, deprotection, lactone hydrolysis, and cation exchange reaction, synthesis of rosuvastatin calcium has been achieved in a one-pot reaction in an excellent overall yield and without any detectable epimerization. This new convergent route, which is also free of any steps which require cryogenic conditions, is superior to other methods for the preparation of rosuvastatin (ČASAR, Zdenko, STEINBÜCHER, Miha, KOŠMRLJ, Janez, *J. Org. Chem.* 2010, *75*, 6681). This article was listed among the journal's top "20 most read articles in October 2010" and highlighted in "Highlights from the Literature" in *Organic Process Research & Development* 2010, *14*, 1276. For the preparation of the key heterocyclic intermediate, employed for the synthesis of rosuvastatin, according to the above methodology, we filed a patent application.

A series of pyrazolone-fused combretastatins and precursors were synthesized and their cytotoxicity as well as antitubulin potential were evaluated. One of the hydrazides, namely, a precursor to pyrazolone-fused combretastatin containing 2-naphthyl substituents as well as three pyrazolone-fused combretastatins, were highly cytotoxic against various tumor cell lines including cisplatin resistant cells. The same compounds were also the best inhibitors of tubulin polymerization. The results of molecular modeling showed that they bind the colchicine binding site at the tubulin heterodimer. The above-mentioned hydrazide arrested HeLa cells in the G2/M phase of the cell cycle and strongly affected the cell shape and microtubule network. (BURJA, Bojan, ČIMBORA, Tamara, TOMIĆ, Sanja, JELUŠIĆ, Tihana, KOČEVAR, Marijan, POLANC, Slovenko, OSMAK, Maja, *Bioorg. Med. Chem.* 2010, *18*, 2375).

Possibilities of extending [^{18}F]-FDDNP PET application from the diagnosis of Alzheimer's to other neurodegenerative diseases in which characteristic protein aggregation in the CNS is present were evaluated through joint cooperation between the research groups from the University of California at Los Angeles, Indiana University, and School of Medicine, University of Ljubljana. Such pathology is also found in the CNS of patients with a rare Gerstmann-Sträussler-Scheinker disease. We reported on our study in which six symptomatic and asymptomatic carriers of PRNP mutations were tested using [^{18}F]-FDDNP PET, [^{18}F]-FDG PET, and MRI together with *in vitro* autoradiography of the brain specimen with [^{18}F]-FDDNP. The results indicate that the synthesized molecular probe [^{18}F]-FDDNP enables successful detection of changes in the CNS of patients with PRNP mutation with PET and suggested that the methodology could be used to monitor the progression therapeutic interventions. (KEPE, Vladimir, GHETTI, Bernardino, FARLOW, Martin R., BRESJANAC, Mara, MILLER, Karen, HUANG, Sung-Cheng, WONG, Koon-Pong, MURRELL, Jill Renee, PICCARDO, Pedro, EPPERSON, Francine, REPOVŠ, Grega, ŠMID, Lojze, PETRIČ, Andrej, SIDDARTH, Prabha, LIU, Jie, SATYAMURTHY, Nagichettiar, SMALL, Gary W., BARRIO, Jorge R. *Brain Pathol.* 2010, *20*, 419).

Propargyl functionalized diazenes were prepared by two different approaches and were examined as alkyne click components in copper(I)-catalyzed azide-alkyne cycloadditions with 2-(azidomethyl)pyridine and four α-azido-ω-aminoalkanes (C2 to C5). While the reactions with α-azido-ω-aminoalkanes reached completion with copper(II) sulphate without the need of reducing agent typically in no more than few minutes, 2-(azidomethyl)pyridine required the addition of metallic copper and much longer reaction times (2–24 h). This difference in the reactivity was studied and a plausible mechanism was proposed (URANKAR, Damijana, STEINBÜCHER, Miha, KOSJEK, Jaka, KOŠMRLJ, Janez, *Tetrahedron* 2010, *66*, 2602).

An alternative, i.e. mild and highly efficient synthetic approach to platinum complexes with bioactive carrier ligands has been developed. It is based on a platinum-complex-tolerant copper(I)-catalyzed 1,3-dipolar cycloaddition between terminal acetylene and a platinum complex that is already functionalized with an azido moiety. As demonstrated by the preparation of novel diazenecarboxamide-carboplatin conjugates, this approach is superior to other methodologies (URANKAR, Damijana, KOŠMRLJ, Janez, *Inorg. Chim. Acta* 2010, *363*, 3817).

We have demonstrated experimentally and theoretically how N2 nitrogen atom of a 1,2,3-triazole ("click triazole") can actively participate in coordination with different transition metal ions, including Pt(II), Pd(II), Cu(II), Ru(II), Ag(I). Thus, we prepared a model compound 1-(2-picolyl)-4-phenyl-1*H*-1,2,3-triazole (**L**). Coordination to the metal ions was investigated with *cis*-$[PtCl_2(DMSO)_2]$, $[Pd(CH_3CN)_4](BF_4)_2$, $CuCl_2$, $[RuCl(\mu\text{-}Cl)(\eta^6\text{-}p\text{-cymene})]_2$ and $AgNO_3$, to give stable chelates $[PtCl_2\mathbf{L}]$, $[Pd(\mathbf{L})_2](BF_4)_2$, $[CuCl_2(\mathbf{L})_2]$, $[RuCl(\eta^6\text{-}p\text{-cymene})\mathbf{L}]OTf$ and $[Ag_2(\mathbf{L})_2(NO_3)_2]$, respectively, with 60–98% yield. The structures of the chelates were unambiguously confirmed by NMR spectroscopy and single crystal X-ray diffraction analysis. Our theoretical study revealed that the stabilization of the resulting coordination compounds is mostly due to π-back-donation from the metal to the aromatic ligand, and to a lesser extent due to electrostatic interactions, as previously reported in literature (URANKAR, Damijana, PINTER, Balazs, PEVEC, Andrej, DE PROFT, Frank, TUREL, Iztok, KOŠMRLJ, Janez, *Inorg. Chem.* 2010, *49*, 4820).

1-Picolyl-1,2,3-triazole has been identified as a ligand with a versatile coordination ability, allowing mono-, bi- and polidentate coordination to different metal ions, including those of rhodium, gold, palladium and mercury. This has been demonstrated by a model compound 1-(2-picolyl)-4-phenyl-1*H*-1,2,3-triazole (**L**) and its complexes: $[Rh_2(O_2CCH_3)_4(\mathbf{L})_2]$, $[PdCl_3(H\mathbf{L})]\cdot H_2O$, $(H\mathbf{L})_2[AuCl_4]Cl$ and $[Hg_4Br_8(\mathbf{L})_2]_n$. The structures of these compounds were determined by single crystal X-ray diffraction analyses. In the rhodium complex ligand **L** coordinates monodentately through the pyridyl N4 atom to the axial site of Rh. In the palladium compound N4 is a protonated ligand **L**, which is coordinated triazole N3 nitrogen atom. The ionic gold compound is composed of three types of ions, $H\mathbf{L}^+$, $AuCl_4^-$ and Cl^-, interconnected by hydrogen bonds. The mercury complex is a coordination polymer in which two **L** ligands stabilize the Hg_4Br_8 chain, and the coordination involves N2 and N3 nitrogen atoms of the triazole and the pyridyl nitrogen atom N4. It has been shown that this ligand enables different supramolecular associations through hydrogen-bonding, C–H•••π and π–π stacking interactions (URANKAR, Damijana, PEVEC, Andrej, TUREL, Iztok, KOŠMRLJ, Janez, *Cryst. Growth Des.* 2010, *10*, 4920). This article was listed among the journal's top "20 most read articles in November 2010".

A comparative study for a selective glucosylation of *N*-unsubstituted 4-hydroxyquinolin-2(1*H*)-ones into 4-(tetra-*O*-acetyl-β-D-glucopyranosyloxy)quinolin-2(1*H*)-ones has been performed. Four glycosyl donors were tested, along with different promoters and reaction conditions. The best results were obtained with tetra-*O*-acetyl-*α*-D-glucopyranosyl bromide with Cs_2CO_3 in CH_3CN. In some cases the 4-*O*-glucosylation of the quinolinone ring was accompanied by 2-*O*-glucosylation, yielding the corresponding 2,4-bis(tetra-*O*-acetyl-β-D-glucopyranosyloxy)quinoline. During deacetylation with Et_3N in MeOH, yielding 4-(β-D-glucopyranosyloxy)quinolin-2(1*H*)-ones, the sugar–aglycon bond cleavage was observed in some cases (KIMMEL, Roman, KAFKA, Stanislav, KOŠMRLJ, Janez, *Carbohydr. Res.* 2010, *345*, 768). The structure of one of the above mentioned products was studied by a single crystal X-ray diffraction analysis (KIMMEL, Roman, NEČAS, Marek, KAFKA, Stanislav, KOŠMRLJ, Janez, VÍCHA, Robert, *Acta Crystallographica. E, Structure Reports* 2010, *E66*, o1328).

Our research has brought forward new knowledge on the synthesis of complex compounds, especially on the synthesis of novel types of building-blocks and on the development of new synthetic methods. Novel reactions in organic synthesis have been thoroughly investigated and explained. In addition to that, we have also synthesized some new biologically active compounds; some of which proved to be suitable for detecting certain diseases.

OTHER RELEVANT ACHIEVEMENTS

INTERNATIONAL PATENT

– ANDERS, Manfred, LICHTBLAU, Dirk Andreas, KOLAR, Jana, MALEŠIČ, Jasna, STRLIČ, Matija, ŠALA, Martin, KOČEVAR, Marijan. *Antioxidant for an organic material and method for treating the same : patent : EP 1664431 (B1), 2010-08-04*. [S. l.]: European Patent Office, 2010. 21 pages.

In our investigations within the 5th FP project InkCor, EVKA4-CT-2001-00049 (coordinator J. Kolar) we were interested in the inhibition of iron-gall-ink corrosion. This investigation resulted in an international patent application (in 2005); in 2010 the EU patent was assigned to this application. In our laboratory two target compounds (myo-inositol phosphates) were prepared; they were shown to prevent iron-gall-ink decay in cellulose items at the same level as phytic acid dodecasodium salt. As such they can serve as a tool for stabilizing paper documents.

PATENT APPLICATIONS

1. OSMAK, Maja, POLANC, Slovenko, ČIMBORA, Tamara, BROZOVIĆ, A., KOČEVAR, Marijan, MAJCE, Vita, ALIČ, Branko. *Analogues of 1,3-bis(4-nitrophenyl)triazenes, their pharmaceutically acceptable salts and N-acyl derivatives for tumor treatment : patent application: WO 2010103338 (A1), 2010-09-16*. [S. l.]: World Intellectual Property Organization, 2010. 21 pages.

   Cancer treatment requires new efficient drugs for a successful chemotherapy. Our patent application refers to analogs of 1,3-bis(4-nitrophenyl)triazenes, their pharmaceutically acceptable salts and *N*-acyl derivatives as promising candidates to develop new drugs for the treatment of cancer patients. These compounds are cytotoxic in very low concentrations (IC50 0.22 to 12.8 μM), and are well soluble. Our investigations indicate that the above-mentioned compounds could be used in the treatment of cancer patients alone or in a combination with other anti-cancer drugs.

2. ČASAR, Zdenko, KOŠMRLJ, Janez. *Key intermediates for the synthesis of rosuvastatin or pharmaceutically acceptable salts thereof : international application no.: WO 2010/086438 A1*. [S. l.]: World Intellectual Property Organization, International Bureau, 5.08.2010. 40 pages.

   This patent application relates to the preparation of *N*-(4-(4-fluorophenyl)-6-isopropyl-5-methylpyrimidin-2-yl)-*N*-methylmethanesulfonamide, *N*-(5-(bromomethyl)-4-(4-fluorophenyl)-6-isopropylpyrimidin-2-yl)-*N*-methylmethanesulfonamide and *N*-(4-(4-fluorophenyl)-5-(hydroxymethyl)-6--isopropylpyrimidin-2-yl)-*N*-methylmethanesulfonamide, key intermediates in the preparation of Rosuvastatin.

3. KIDEMET, Davor, ZUPET, Rok, SMODIŠ, Janez, ŠTEFANE, Bogdan, POŽGAN, Franc. *Process and intermediates for the preparation of aliskiren : Application No. 09176568.5-1211*. Rijswijk: European Patent Office, 11. 1. 2010.

4. TUREL, Iztok, KLJUN, Jakob, ŠTEFANE, Bogdan. *Postopek za pripravo racemnega nikotina : št. P-201000450*. Ljubljana: Urad Republike Slovenije za intelekturalno lastnino, 22.12.2010. 7 pages.

INTERNATIONAL AWARD

Assist. Prof. Bogdan Štefane was awarded a prestigious Fulbright scholarship. From October 2009 to March 2010 he was a visiting scholar at the University of Maryland, USA, where he conducted research in the field of signaling pathways of bacterial virulence. His research was published in two outstanding publications (one in 2011):

1. WANG, Jingxin, ŠTEFANE, Bogdan, JABER, Deana, SMITH, Jacqueline A. I., VICKERY, Christopher, DIOP, Mouhamed, SINTIM, Herman O. Remote C-H functionalization: using the N-O moiety as a atom-economical tether to obtain 1,5- and the rare 1,7-C-H insertions. *Angew. Chem. (Int. ed., Print)* 2010, *49*, 3964.
2. NAKAYAMA, Shizuka, KELSEY, Ilana, WANG, Jingxin, ROELOFS, Kevin, ŠTEFANE, Bogdan, LUO, Yiling, LEE, Vincent T., SINTIM, Herman O. Thiazole orange-induced c-di-GMP quadruplex formation facilitates a simple fluorescent detection of this ubiquitous biofilm regulating molecule. *J. Am. Chem. Soc.* 2011, *133*, 4856.

PLENARY AND INVITED LECTURES

Several plenary and invited lectures were delivered at international conferences and one invited lecture at a national conference.

OTHER ACTIVITIES AND RECOGNITIONS

M. Kočevar is a member of the Management Committee COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011).

Upon the invitation of Professor Jun-Il Jin, the President of IUPAC, M. Kočevar became IUPAC Fellow as of 2010 (See: http://www.iupac.org/web/per/kocevar).

Editorial activity: K. Kranjc is a member of the editorial board (2007−) of the *Acta Chimica Slovenica* (ACSi), M. Kočevar is a member of the editorial board of the *Periodica Polytechnica. Chemical Engineering* (2003−); S. Polanc is a member of the editorial board of the *Topics in Heterocyclic Chemistry* (2008−).

Members of our research group, Andrej Petrič, Bogdan Štefane, and Franc Požgan, partly participate in the EN-FIST Centre of Excellence (CO EN-FIST; http://enfist.si/). R&D project “Compounds for diagnostics and medical therapy” aims towards utilization of modern synthetic approaches, such as metathesis and cross coupling reactions, in the synthesis of new and known pharmaceuticals as well as in the synthesis of novel molecular probes for medical research and diagnostics.

A member of our research group, Andrej Petrič, is heading the Center for NMR spectroscopy at UL FKKT (http://nmr-slave.fkkt.uni-lj.si). Together with another member of the research group, Janez Košmrlj, they have organized maintenance and utilization of the existing, 15-year-old 300 MHz NMR instrument, and put efforts into the acquisition of two new NMR instruments, co-financed by the ARRS through the 14th package programme. One of the in-

struments is installed at the Faculty of Chemistry and Chemical Technology, and the other at the Faculty of Pharmacy. Both instruments have been in operation since December 2010. The research results which were supported by the activities of the NMR Center were published in 60 original and review scientific papers, ten invited lectures were delivered, 89 contributions at scientific meetings, one patent, and 5 patent applications. The services were utilized also for the research work in the preparation of eight doctoral, two master's, and 28 diploma theses.

Members of the research group Janez Košmrlj and Andrej Petrič have taken actions to acquire a new Agilent 6224 Accurate Mass TOF LC/MS instrument, financed by the Faculty of Chemistry and Chemical Technology. Hopefully, the instrument will start providing services in January 2011.

Our group has also collaborated in some bilateral projects with Argentina, Croatia, Czech Republic and Romania and led several industrial and other projects.

KEMIJSKO INŽENIRSTVO
CHEMICAL ENGINEERING

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P2–0191

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Matjaž Krajnc

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
prof. dr. Aleksander Pavko
prof. dr. Marin Berovič
prof. dr. Igor Plazl
izr. prof. dr. Jana Zagorc Končan
doc. dr. Ana Lakota
doc. dr. Urška Šebenik
doc. dr. Andreja Zupančič Valant
doc. dr. Polona Žnidaršič Plazl
doc. dr. Andreja Žgajnar Gotvajn
doc. dr. Mitja Lakner

Mladi raziskovalci / Young Researchers
Janja Babič
Mirjan Švagelj
Andrej Pohar
Matjaž Berlot
Ervin Šinkovec
Martin Lubej
Uroš Novak

Strokovni sodelavec / Research Assistant
Branko Alič, univ. dipl. kem.

Tehniki / Technicians
Vesna Delalut
Klemen Birtič
Janez Malovrh

Sodelujoče institucije / Participating Institutions
UL, Fakulteta za gradbeništvo in geodezijo

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Vsebinsko izhodišče programa Kemijsko inženirstvo je študij transportnih pojavov v heterogenih reakcijsko-difuzijskih sistemih, ki vključuje matematično-fizikalni zapis procesov na različnih nivojih opazovanja od molekularnega do makroskopskega, razvoj nelinearnih sistemov za opis procesov ter razvoj produktov za aplikacije, ki zahtevajo podrobno poznavanje kompleksnih transportnih mehanizmov. Raziskovalni program ja zasnovan tako, da omogoča integriran multidisciplinaren sistematičen pristop, s katerim bo mogoče razvijati osnovna kemijsko inženirska znanja in jih aplicirati na specifičnih kemijsko inženirskih področjih. Cilji programa so opredeljeni po delitvi vsebine programa na specifična kemijsko inženirska področja, ki so: *kemijsko procesno inženirstvo z reologijo, polimerno inženirstvo, biokemijsko inženirstvo* in *ekološko inženirstvo.*

KEMIJSKO PROCESNO INŽENIRSTVO Z REOLOGIJO

Mikrotehnologija predstavlja pomemben dejavnik razvoja na številnih področjih, od industrije elektronike, proizvodnje gorivnih celic, do farmacevtske in kemijske industrije, medicinske tehnologije, biotehnologije in okoljevarstva. Vpeljava mikroreaktorjev v (bio)kemijske procese v zadnjih letih zavzema precejšnjo pozornost, predvsem zaradi majhne porabe kemikalij in zelo učinkovitega prenosa toplote in snovi kot posledice visokega razmerja med površino in volumnom reaktorjev, lažjega nadzora procesnih pogojev in novega koncepta postavitve proizvodnje na osnovi povečanja števila enot (numbering-up) namesto klasičnega povečevanja (scale-up). V sklopu raziskav študiramo mikrofluidne pojave in reakcijsko-difuzijsko dinamiko različnih (bio)kemijskih procesov v mikrostrukturiranih napravah. Pridobljeno znanje bomo uporabili pri razvoju integriranih »lab-on-a-chip« sistemov.

Večfazni sistemi zavzemajo pomembno vlogo v večini proizvodnih procesov. Visoka stopnja znanja pri načrtovanju izbrane naprave je ključnega pomena za njeno optimalno delovanje tako glede kvalitete produkcije kot ekonomike proizvodnje na okolju prijazen način. Glede na stopnjo izbranega kontrolnega volumna načrtovanje multifaznega sistema sloni na sofisticiranem numeričnem reševanju bilanc transportnih količin ali na postavitvi fenomenoloških modelov, ki bazirajo na eksperimentalnem opazovanju tokovne slike. Končni cilj je verodostojna napoved fluidne dinamike in transporta ter kinetično-adsorbcijskih pojavov v odvisnosti od operativnih parametrov. Kljub hitremu razvoju dosegljivih matematičnih orodij, ki omogočajo simulacijo tokovnih oblik v velikih napravah, je eksperimentalna verifikacija tista, ki potrdi

pravilnost izbire zaprtja (enclosure) sistema. Ne-newtonski mediji so z svojo kompleksno reološko sliko prisotni v večini procesov v bio-proizvodnji, vendar kljub temu v odprti literaturi primanjkuje eksperimentalnih študij o njihovem vplivu na performanco aparature. Smernice: v primeru ne-newtonskih medijev s poudarjeno elastično komponento se je pokazala izredno kompleksna slika hidrodinamskega dogajanja v koloni, ki jo je težko podvreči volumskemu ali časovnemu povprečenju, kar je običajno pri razvoju manjparametrskih zveznih ali stopenjskih modelov. Zato je potrebno raziskave usmeriti v pridobivanje lokalnih vrednosti hidrodinamskih parametrov in snovnega transporta, ter tako ustvariti podatkovno bazo za razvoj večparametrskega modela celic in pristop s CFD metodo.

V izolacijskem postopku farmacevtskih učinkovin predstavlja pomembno fazo koncentriranje vodne raztopine produkta. Ena izmed možnosti je uparjanje, ki se zaradi morebitne termične nestabilnosti produkta lahko izvaja pri nižjih tlakih, vendar jo zaradi nižjih investicijskih in obratovalnih stroškov upravičeno nadomeščajo membranske separacije, ki jo lahko izvajamo pri nizkih temperaturah. V zadnjem času se raziskave in aplikacije koncentriranja s pomočjo membranskih operacij intenzivirajo tudi na sistemih raztopin z organskimi topili. V literaturi najdemo nekaj modelov transporta snovi skozi membrano, ki upoštevajo na primer porozno strukturo membrane, ‘raztapljanje’ topila v membrani, model zaporednih uporov ter površinske napetosti membrane in topila. Z izbiro industrijsko uporabnih topil in učinkovin ter določanjem fluksov in zadrževalnih faktorjev pri različnih obratovalnih pogojih so raziskave aplikativno naravnane. Vendar so po svoji vsebini tudi temeljne, ker poskušajo najti razlago za transport topila in separacijo topljenca s pomočjo obstoječih modelov ali postavitvijo novega modela. Poudarek raziskav je v laminarnem sloju ob membrani na strani koncentrata in interakciji membrana-topilo-topljenec. Cilj raziskav je izračun potrebne površine membran za izbrane obratovalne pogoje in ekonomska primerjava nanofiltracije z uparjanjem.

Poznavanje pretočnosti reološko kompleksnih tekočin je pomembno pri razumevanju tehnoloških procesov v katerih le te nastopajo kot procesne tekočine, ali kot produkti. Realne tekočine (heterogeni sistemi) so ne-newtonske, ker izkazujejo različne odzive na delovanje strižnih sil in strižni tok. Vzrok je kompleksna notranja struktura materiala (tekočine), ki je odvisna od molekularnih interakcij in kombinacije delovanja privlačnih in odbojnih sil med posameznimi komponentami heterogenega sistema. Kot notranjo strukturo materiala lahko smatramo že samo konfiguracijo polimernih molekul, v heterogenih sistemih pa poleg primarnih molekularnih lastnosti tudi sestavo, vsebnost in kompatibilnost osnovnih lastnosti posameznih komponent. Zaradi delovanja sil v strižnem toku, se reološko kompleksne snovi odzivajo ne-izotropno, zato izkazujejo viskoelastične lastnosti. Pri proučevanju reoloških lastnosti se pogosto poslužujemo fenomenoloških pristopov. To pomeni, da na osnovi reološke karakterizacije, določene iz eksperimentalnih podatkov pri različnih strižnih pogojih, določimo materialne funkcije, iz katerih lahko sklepamo na fizikalno-kemijske vplive posameznih komponent v sistemu. Pri raziskovalnem delu preučujemo reološke lastnosti heterogenih polimernih talin z namenom določiti ključne dejavnike sestave, ki vplivajo na mehanske lastnosti polimernih materialov. Na osnovi eksperimentalnih podatkov določamo reološke modele (konstitutivne enačbe stanja) za opis strižno odvisnega obnašanja polimernih talin različne sestave. Na ta način bomo določili primerno formulacijo polimernega materiala, ki bo izkazovala zahtevane lastnosti in proučili transportne parametre notranje strukture heterogenih sistemov.

Poznavanje pretočnosti krvi, kardioplegičnih in fizioloških raztopin je pomembno pri razumevanju delovanja kardiovaskularnih sistemov pri normalnih pogojih in v obolelosti. Za natančen opis hidrodinamskega obnašanja krvi in modelnih telesnih tekočin je treba določiti primeren reološki model, ki podaja odvisnost viskoznosti tekočine od strižne hitrosti v širokem območju strižnih hitrosti. V okviru raziskovalnega dela iz izmerjenih eksperimentalnih podatkov dolo-

čamo reološke modele za opis strižno odvisnega obnašanja krvi, kardioplegičnih raztopin in modelnih telesnih tekočin in njihovo temperaturno odvisnost. Na osnovi poznavanja reologije krvi opredeljujemo učinek različnih dodatkov (volumski ekspanderji in drugi polisaharidi) na tokovno obnašanje modelnih telesnih tekočin pri različnih temperaturnih režimih. Konstitutivne enačbe za opis strižno odvisnega obnašanja preučevanih telesnih tekočin, ki vsebujejo temperaturno odvisne materialne parametre, uporabljamo pri simulaciji pretoka v 2D in 3D geometrijah. Rezultati simulacij lahko vodijo k izboljšanju nekaterih sestavin modelnih telesnih tekočin in k njihovi optimalni rabi v praksi. Numerične simulacije pretočnosti in tokov proučevanih raztopin in krvi v realnih geometrijah kot so koronarne žile in srčne poti pri različnih temperaturnih režimih dajejo koristne informacije v kirurgiji srca.

POLIMERNO INŽENIRSTVO

Mikroinkapsulacija je proces, s katerim se drobni delci ali kapljice obdajo z ovojem, kar daje kapsulam majhnih dimenzij številne uporabne lastnosti. Material, ki se nahaja v notranjosti kapsul, imenujemo jedro, notranja faza ali polnilo, medtem ko material ki obdaja jedro, imenujemo lupina, ovoj ali membrana. Razlogov za mikroinkapsulacijo je mnogo. V nekaterih primerih jedro izoliramo od njegove okolice in tako preprečimo izhlapevanje lahkohlapnega materiala, izboljšamo ali omogočimo rokovanje z lepljivimi materiali ali pa preprečimo kemijsko reakcijo reaktivnega jedra. V drugih primerih pa želimo nadzorovati hitrost transporta učinkovin (npr.: zdravilne učinkovine, pesticidi,…) iz jedra preko membrane. Razlogi so lahko različni, od tako preprostih, kot je prekrivanje okusa ali vonja jedra, do tako kompleksih, kot je povečana selektivnost procesa adsorpcije ali ekstrakcije. Cilj raziskovalnega programa je razvoj metod mikroinkapsulacije različnih materialov, ki predstavljajo jedro, s polimernimi ovoji. Raziskujemo polimerizacijski proces, s katerim nastaja ovoj. Aplikativne lastnosti mikrokapsul raziskujemo z različnimi tehnikami, tudi s študijo prenosa snovi iz jedra preko polimerne membrane v okolico.

PSA (»Pressure Sensitive Adhesives«) so lepila občutljiva na pritisk. Med PSA lepila spadajo materiali, ki imajo agresivno in trajno začetno adhezijo, se prilepijo z uporabo pritiska prsta, ne potrebujejo aktivacijske energije za tvorbo vezi in imajo zadostno kohezijo za omogočanje enostavne odstranitve nosilca iz površine materiala (brez vidnih ostankov adheziva). Za sintezo PSA lepil se na svetovnem trgu v veliki meri uporabljajo akrilatni monomeri, katerih polimeri imajo edinstvene lastnosti. Glede na vrsto uporabljene tehnologije za pridobitev končnega produkta razdelimo PSA lepila na: lepila na osnovi organskih topil, lepila na vodni osnovi (emulzije in suspenzije), lepila v talini (»hot melt« lepila) in radiacijsko zamrežljiva lepila. V prvem delu raziskav študiramo suspenzijsko polimerizacijo, s katero nastajajo mikrosferna PSA lepila na vodni osnovi. Cilj je razvoj metode in procesa za sintezo produkta želenih lastnosti. Raziskave vključujejo razvoj novega nanokompozitnega PSA lepila. Drugi cilj raziskav je razvoj prav tako novega, komercialno uporabnega radiacijsko zamrežljivega PSA akrilatnega lepila, ki se lahko nanaša na substrat in se zamrežuje pri sobni temperaturi s pomočjo UV sevanja. Vzporedno raziskujemo prenos toplote med polimerizacijo akrilatnih monomerov v masi.

Raziskujemo sintezo polisiloksanskih emulzij z emulzijsko polimerizacijo po anionskem mehanizmu z odpiranjem monomernega obroča. Cilj je preučiti vpliv sestave in reakcijskih parametrov na končne lastnosti emulzij ter pri tem raziskati zelo kompleksen mehanizem sinteze.

Preučujemo kinetiko sinteze in zamreževanja formaldehidnih smol s ciljem optimizirati proizvodni postopek sečninsko-formaldehidnih smol in razviti tehnologijo priprave melaminskih pen.

Študirali smo kinetiko vulkanizacije in prenos toplote med vulkanizacijo izbranih mešanic kavčukov. Procesa smo opisali z matematičnim modeliranjem. Pripravili smo nove gumene nanokompozite in raziskovali ter modelirali njihove viskoelastične lastnosti v širokem razponu temperatur in frekvenc. Določali smo tudi druge relevantne lastnosti nanokompozitnih materialov in jih povezali s sestavo in strukturo materiala.

BIOKEMIJSKO INŽENIRSTVO

Biotransformacije in biodegradacije kemijskih spojin naravnega ali umetnega izvora se uporabljajo v številnih kemijskih, farmacevtskih in živilskih industrijah, ter še posebno v proizvodnji finih kemikalij ter pri zaščiti okolja. Med glavne cilje področja sodi načrtovanje procesov z imobiliziranimi encimi ali celotnimi celicami, ki jih lahko ponovno uporabljamo vse dokler ostanejo aktivni, s čimer minimiziramo stroške ter omogočimo ekonomsko ugodnejši kontinuirni način obratovanja. Nadaljnja integracija procesov z drugimi kemijskimi procesi ter z zaključnimi procesi bi omogočila zelo učinkovite in okolju prijazne proizvodnje. Povezava biokatalitskih procesov z mikroreaktorsko tehnologijo predstavlja velik potencial razvoja na tem področju. V zadnjih letih precej študij obravnava razvoj encimskih mikroreaktorjev in njihova uporaba je v glavnem usmerjena v kemijsko analizo in kinetične študije. V okviru raziskovalnega programa nameravamo razvijati kontinuirne procese izbranih biotransformacij v mikroreaktorjih z uporabo imobiliziranih celic ali encimov z integriranim ločevanjem produktov. Razvoj mikroreaktorske tehnologije je osnovan na uporabi povezave med nanotehnologijo in ionskimi kapljevinami, ki v zadnjem času pritegujejo pozornost kot »zelena« topila v organskih sintezah ter še posebno v katalitskih procesih. Nedavno se je uporaba ionskih kapljevin kot reakcijskega medija razširila tudi na encimsko katalizo in biotransformacije s celotnimi celicami, vendar pa je njihova uporaba v industrijskem merilu zelo omejena zaradi visokih cen na trgu. Zaradi tega je razvoj procesov s temi topili na mikro nivoju obetavna alternativa.

Raziskujemo vpliv transportnih pojavov v reološko spremenljivih medijih v heterogenem reakcijsko-difuzijskem sistemu kultivacije basidiomicet in njihov vpliv na razvoj farmacevtsko aktivnih produktov, polisaharidov in proteinov v smislu produkcije proti tumornih, proti rakavih in imunostimulatornih učinkovin, ter njihov vpliv na tehnologijo produkcije, izolacije in purifikacije aktivnih komponent, njihovo testiranje in vitro in izdelavo tržnih produktov za uporabo v veterini in humani medicini v smislu zdravil brez receptov.

EKOLOŠKO INŽENIRSTVO

Uporabna biokataliza je relativno mlada znanost, ki si skozi bioremediacijo utira pot na področje ekološkega inženirstva. Encimi in mikroorganizmi so namreč zanimivi za ekološko prijazno reševanje problema industrijskih odplak z organskimi polutanti. V zadnjem desetletju se je močno povečalo zanimanje za možnost bioremediacije s pomočjo gliv bele trohnobe, ki razgradnjo organskih aromatskih polutantov povzročajo z značilnimi lignin peroksidaznimi, mangan peroksidaznimi in lakaznimi aktivnostimi, posebno če rastejo v imobilizirani obliki na ustreznem nosilcu. Na aktivnosti vezanih in prostih encimov je mogoče vplivati z izbiro primernega gojišča ter nosilca in načinom gojenja oziroma vodenja procesa. Izkušnje kažejo, da je v te namene najprimernejši reaktor z rotirajočimi diski. Raziskave obsegajo študije vpliva sestave gojišča in vpliva vrste nosilca na specifične encimske aktivnosti in hitrosti razgradnje izbranih organskih polutantov, predvidoma organskih barvil. Primarni cilj je pridobiti nova spoznanja o potencialni uporabnosti gliv in encimov pri ekološko prijaznem načinu reševanja problema organskih industrijskih odplak z bioremediacijo. Iz ekonomskega aspekta je razgradnja pod nesterilnimi pogoji cenejša, zato je zanimiva primerjava učinkovitosti procesa pri

sterilnih oziroma nesterilnih pogojih. Cilj je tudi preizkus uporabnosti tehnologije na realnih vzorcih odpadnih vod in v perspektivi prenos v industrijsko prakso.

OSREDNJE TEME PROGRAMA

Kemijsko procesno inženirstvo z reologijo

- Mikroreaktorska tehnologija
- Desorpcija kovin iz prsti v kontinuirnem sistemu
- Eksperimentalni študij hidrodinamskih in kinetično-adsorpcijskih parametrov kolone z ekspandiranim slojem
- Izolacija aktivnih farmacevtskih učinkovin
- Reološko kompleksne tekočine

Polimerno inženirstvo

- Raziskave na področju mikroinkapsulacije
- Sinteza, karakterizacija in optimizacija procesa sinteze akrilatnih lepil
- Sinteza, priprava in karakterizacija nanokompozitnih materialov
- Sinteza, karakterizacija in optimizacija procesa sinteze polisiloksanskih emulzij
- Sinteza, karakterizacija in optimizacija procesa sinteze različnih formeldehidnih smol
- Raziskave na področju tehnologije priprave melaminskih pen
- Študij kinetike vulkanizacije različnih gumenih zmesi in modeliranje
- Študij prenosa toplote med vulkanizacijo različnih gumenih zmesi in modeliranje
- Mehanskih lastnosti gume in gumenih kompozitov

Biokemijsko inženirstvo

- Kontinuirni proces biotransformacije steroidov
- Ekstrakcija steroidov v mikroreaktorju
- Biokatalitske reakcije v mikroreaktorju
- Študij encimsko katalizirane sinteze izoamil acetata
- Optimizacija tehnološkega postopka vodenja kultivacije farmacevtsko aktivne glivine biomase
- Biosinteze ekstra in intracelularnih učinkovin s submerzno kultivacijo in kultivacijo glivine biomase na trdnem gojišču
- Gojenje *Grifole frondose* na sekundarnih surovinah kmetijske in lesno predelovalne industrije na eksperimentalni farmi gob
- Izolacija in purifikacija glivinih polisaharidov
- Testiranje aktivnosti indukcije citokinov na človeških celičnih linijah

Ekološko inženirstvo:

- Raziskave na področju bioremediacije
- Nitrifikacija v biološkem reaktorju s pritrjeno biomaso
- Biološki in fizikalno-kemijski postopki čiščenja odpadnih vod
- Napredni oksidacijski procesi za odstranjevanje biološko stabilnih nevarnih organskih onesnaževal iz odpadnih vod

– Razvoj novih kroničnih strupenostnih testov z organizmom Artemia salina
– Razvoj strupenostnih testov z višjimi rastlinami z merjenjem encimskih odzivov
– Okoljski vplivi različnih ionskih tekočin kot sodobnih topil in reakcijskih medijev

ZNANSTVENI DOSEŽKI

Mikroreaktorska tehnologija: Mikrotehnologija predstavlja pomemben dejavnik razvoja na številnih področjih, od industrije elektronike, proizvodnje gorivnih celic, do farmacevtske in kemijske industrije, medicinske tehnologije, biotehnologije in okoljevarstva. Vpeljava mikroreaktorjev v (bio)kemijske procese v zadnjih letih zavzema precejšnjo pozornost, predvsem zaradi majhne porabe kemikalij in zelo učinkovitega prenosa toplote in snovi kot posledice visokega razmerja med površino in volumnom reaktorjev, lažjega nadzora procesnih pogojev in novega koncepta postavitve proizvodnje na osnovi povečanja števila enot (numbering-up) namesto klasičnega povečevanja (scale-up). V okviru raziskav smo preučevali različne homogene in heterogene sisteme. Objava:

– PLAZL, Igor, LAKNER, Mitja. *Modeling and finite difference numerical analysis of reaction-diffusion dynamics in a microreactor. Acta chim. slov.. [Tiskana izd.], 2010, vol. 57, no. 1, str. 100–109. http://acta.chem-soc.si/57/57-1-100.pdf.* [COBISS.SI-ID 33804805].

Desorpcija kovin iz prsti v kontinuirnem sistemu: V okviru procesnega inženirstva smo proučevali desorpcijo nekaterih elementov (B, Cd, Co, Mn, Ni, and Sr) iz prsti v kontinuirnem sistemu, ki je predstavljal človeški želodec. Eksperimentalne podatke smo razložili z matematičnim modelom. Vzorce prsti (50 mg) iz mesta Cornwall (Anglija) smo kontaktirali z umetni želodčno raztopino pri različnih pretokih do prb. 4 ure. Raztopine smo analizirali z induktivno sklopljeno plazmo z masno spektrometrijo (ICP-MS). Profile luženja smo ovrednostili z matematičnim modelom, ki je vključeval snovni prenos skozi film ter difuzijo v delcih. Sistem parcialnih diferencialnih enačb smo rešili numerično z metodo končnih razlik. Objava:

– BEESTON, Michael Philip, POHAR, Andrej, ELTEREN, Johannes Teun van, PLAZL, Igor, ŠLEJKOVEC, Zdenka, VEBER, Marjan, GLASS, Hylke J. *Assessment of physical leaching processes of some elements in soil upon ingestion by continuous leaching and modeling. Environ. sci. technol.. [Print ed.], 2010, vol. 44, issue 16, str. 6242–6248, doi: 10.1021/es1006725.* [COBISS.SI-ID 4448538].

Reološko kompleksne tekočine: Reologija krvi in hemodinamika. Poznavanje pretočnosti krvi in kardioplegičnih raztopin je pomembno pri razumevanju delovanja kardiovaskularnih sistemov pri normalnih pogojih in v primeru obolelosti. Na osnovi izmerjenih reoloških lastnosti krvi smo določili reološke modele za opis strižno odvisnega obnašanja krvi, kardioplegičnih raztopin in zmesi krvi s kardioplegičnimi raztopinami (volumski ekspanderji) in njihovo temperaturno odvisnost. Opredelili smo učinek različnih volumskih ekspanderjev na tokovno obnašanje krvi. Na osnovi reoloških podatkov smo določili primerne konstitutivne enačbe za opis strižno odvisnega obnašanja krvi različnih donorjev, ki so vsebovale temperaturno odvisne materialne parametre. Le te smo uporabili pri simulaciji pretoka v 3D geometrijah. Raziskovalno delo je potekalo v sodelovanju s kolegi s Cipra (bilateralni projekt), ki so razvili zelo natančne numerične simulacije (high fidelity transient numerical simulation) pretočnosti krvi skozi koronarne žile in srčne poti, z upoštevanjem reoloških modelov, pri različnih temperaturnih režimih. Rezultati simulacij lahko vodijo k izboljšanju nekaterih sestavin v modelnih telesnih tekočinah in k njihovi optimalni uporabi v praksi. Numerične simulacije pretočnosti

in tokov proučevanih raztopin in krvi v realnih geometrijah kot so koromarne žile in srčne poti pri različnih temperaturnih režimih bodo dale koristne informacije v kirurgiji srca. V objavo je sprejet članek:

– ZUPANČIČ-VALANT, Andreja, ŽIBERNA, Lovro, PAPAHARILAOU, Yannis, ANAYIOTOS, Andreas, GEORGIOU, Georgios C. *The influence of temperature on rheological properties of blood mixtures with different volume expanders : implications in numerical arterial hemodynamics simulations. Rheol. Acta, doi: 10.1007/s00397-010-0518-x.* [COBISS.SI-ID 34768133].

Reološko obnašanje gumibitumna kot veziva za proizvodnjo gumiranih asfaltnih zmesi: Raziskovali smo reološke lastnosti gumibitumna. Objava:

– LUKAČ, Bojana, ZUPANČIČ-VALANT, Andreja. *Raziskovanje obnašanja gumibitumna kot veziva za proizvodnjo gumiranih asfaltnih zmesi = The investigation of rubber modified bitumen as a binder for production of asphalt mixtures. Gradb. vestn., 2010, letn. 59, št. 11, str. 261-268.* [COBISS.SI-ID 34588933].

Mikroinkapsulacija: Mikroinkapsulacija je proces ovijanja mikronskih trdnih delcev, kapljic ali mehurčkov v inertno polimerno ovojnico, pri čemer dobimo mikrokapsule s premerom med 1 in 1000 μm, ki so sestavljene iz jedrnega materiala in ovojnega materiala. S pravilno izbiro jedrnega in ovojnega materiala je možno pripraviti mikrokapsule za različna področja uporabe. Proučevali smo in-situ mikroinkapsulacijo z melaminsko-formaldehidnimi smolami. Raziskovali smo vpliv sestave reakcijske zmesi in različnih procesnih parametrov na potek procesa mikroinkapsulacije različnih jedrnih materialov z melaminsko-formaldehidno (MF) smolo v šaržnem reaktorju. Glavna proučevana procesna parametra sta bila (poleg sestave reakcijske zmesi) temperatura in pH vrednost reakcijske zmesi. Z natančnejšo raziskavo vpliva posameznih parametrov na potek mikroinkapsulacije smo ugotavljali vpliv reakcijskih pogojev na lastnosti mikrokapsul oziroma MF stene mikrokapsul, ki določa lastnosti in možno uporabo mikrokapsul. Nadaljujemo z raziskavami inkapsulacije v mikroreaktrorskih sistemih. Rezultati dela raziskav so objavljeni v:

– ALIČ, Branko, ŠEBENIK, Urška, KRAJNC, Matjaž. *Differential scanning calorimetric examination of melamine-formaldehyde microcapsules containing decane. J. appl. polym. sci., 2011, vol. 119, no. 6, str. 3687–3695, doi: 10.1002/app.33077.* [COBISS.SI-ID 34469637].

Sinteza, karakterizacija in optimizacija procesa sinteze akrilatnih lepil: Proučevali smo sintezo ter lastnosti novih UV zamrežljivih akrilatnih mikrosfernih lepil. UV zamrežljiva akrilatna mikrosferna lepila smo sintetizirali s šaržno emulzijsko polimerizacijo z uporabo različnih količin fotoiniciatorjev, ki smo jih uspešno vgradili v polimerno verigo. Dobljena lepila izkazujejo dobre lepilne lastnosti. V naslednji fazi smo pozornost preusmerili na sintezo UV zamrežljivih lepil v masi in sicer po šaržnem in kontinuirnem postopku. Rezultati dela raziskav so objavljeni v:

– KAJTNA, Jernej, KRAJNC, Matjaž. *UV crosslinkable microsphere pressure sensitive adhesives : influence on adhesive properties. Int. j. adhes. adhes.. [Print ed.], 2011, vol. 31, no. 1, str. 29–35, doi: 10.1016/j.ijadhadh.2010.09.004.* [COBISS.SI-ID 34530309].

Sinteza, karakterizacija in optimizacija procesa sinteze polisiloksanskih emulzij: Emulzijska polimerizacija ciklosiloksanov je kompleksen heterogen proces, ki lahko poteka po mehanizmu anionske ali kationske polimerizacije z odpiranjem monomernega obroča. Na potek polimerizacije poleg kemijske kinetike ključno vpliva tudi prenos snovi v kontinuirnem in dispergiranem mediju ter snovni transport med omenjenima fazama. Zaradi kompleksnosti obrav-

navanega sistema ostaja emulzijska polimerizacija ciklosiloksanov predmet številnih raziskav, njen predlagani mehanizem pa je osnovan na številnih hipotezah. Študirali smo vpliv sestave in reakcijskih parametrov na potek emulzijske polimerizacije ciklosiloksanov po mehanizmu anionske polimerizacije z odpiranjem monomernega obroča ter vpliv sestave in reakcijskih parametrov na končne lastnosti polisiloksanskih emulzij. Spremljali smo kinetiko emulzijske polimerizacije, morfologijo delcev, molekulsko maso in porazdelitev molekulske mase polimera ter termične lastnosti polimera (temperatura steklastega prehoda, temperatura tališča, degradacija polimera). Na osnovi rezultatov smo predlagali mehanizem anionske emulzijske polimerizacije ciklosiloksanov, ko je koncentracija emulgatorja nad kritično micelno koncentracijo. Rezultati dela raziskav so objavljeni v:

– MOHORIČ, Ines, ŠEBENIK, Urška. *Anionic ring-opening polymerization of octamethylcyclotetrasiloxane in emulsion above critical micelle concentration. Polymer (Guildf.). [Print ed.], 2011, vol. 52, no. 5, str. 1234–1240, doi: 10.1016/j.polymer.2011.01.025*. [COBISS.SI-ID 34739717].

Mikroreaktorska tehnologija v biokemijskem inženirstvu: Na področju mikroreaktorske tehnologije smo nadaljevali študije različnih biokatalitskih sistemov in separacij. Teoretično in eksperimentalno smo preučili encimsko katalizirano oksidacijo holesterola v kontinuirno delujočem mikroreaktorju. Proces poteka na medfazni površini paralelnega toka *n*-heptana in vodne faze z raztopljeno holesterol oksidazo. Z uravnavanjem pretokov obeh faz smo omogočili vzpostavitev paralelnega toka po sredini mikrokanala in s tem sočasno ločevanje obeh faz na iztoku y-oblikovanega mikroreaktorja. Razvili smo 3D matematični model, ki poleg hitrostnega profila vključuje če konvektivni, difuzijski in reakcijski člen, opisan s kinetiko Michaelisa in Mentenove za dva substrata. Eksperimentalni podatki, ki se dobro ujemajo z teoretičnimi napovedmi, so pokazali 70 % konverzijo pri zadrževalnem času manj kot minuta. V mikrokanalih iz plastičnih materialov in stekla smo uspešno imobilizirali celice kvasovk *Saccharomyces cerevisiae*. Prav tako pa smo uspeli razviti kontinuirni proces biotransformacije progesterona v laboratorijskem bioreaktorju, za katerega smo nato izvedli še kontinuirno ekstrakcijo steroidov v mikrokanalu, kar bi omogočilo postavitev integriranega procesa. Iz omenjenega področja so bili v letu 2010 objavljeni trije članki in en sprejet v objavo:

– MARQUES, M. P. C., FERNANDES, P., CABRAL, Joaquim M. S., ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. *On the feasibility of in-situ steroid biotransformation and product recovery in microchannels. Chem. Eng. J., 2010, 160, 708–714, doi: 10.1016/j.cej.2010.03.056*. [COBISS.SI-ID 33911813].
– STOJKOVIČ, Gorazd, ŽNIDARŠIČ PLAZL, Polona. *Immobilization of yeast cells within microchannels of different materials. Acta chim. slov., 2010, 57, 144–149. http://acta.chem-soc.si/57/57-1-144.pdf*. [COBISS.SI-ID 33807877].
– ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. *Development of a continuous steroid biotransformation process and product extraction within microchannel system. Catal. Today, 2010, 157, 315-320, doi: 10.1016/j.cattod.2010.01.042*. [COBISS.SI-ID 33681925].
– STOJKOVIČ, Gorazd, PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. *L-Malic acid production within a microreactor with surface immobilised fumarase. Microfluid. nanofluid. (Print), 2011, vol. 10, no. 3, str. 627–635, doi: 10.1007/s10404-010-0696-y*. [COBISS.SI-ID 34517509].

Oksidacija koniferil alkohola z grobim pripravkom lakaze: Preučevali smo oksidacijo koniferil alkohola z grobim pripravkom lakaze, ki smo ga pridobili s submerznim gojenjem glive *Trametes versicolor,* ter rezultate primerjali s komerialnim encimom. Za proces smo razvili tudi matematični model, ki smo ga verificirali s serijo eksperimentalnih podatkov. Objava:

– TIŠMA, Marina, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor, VASIĆ-RAČKI, Đurđa, ZELIĆ, Bruno. *Oxidation of coniferyl alcohol catalyzed by laccases from Trametes versicolor. Acta chim. slov. 2010, 57, 110-117. http://acta.chem-soc.si/57/57-1-110.pdf.* [COBISS.SI-ID 33807109].

Prenos kisika v laboratorijskem mešalnem reaktorju med gojenjem celičnih kultur: V laboratorijskem mešalnem bioreaktorju volumna 5 L smo proučevali vpliv vnosa moči z mešali na volumenski koeficient prenosa kisika kLa med gojenjem rekombinantnih sesalskih celic, ki zahtevajo neintenzivno mešanje in prezračevanje. Ugotovili smo, da pri teh obratovalnih pogojih in visoki koncentraciji celic dobava kisika z zrakom ne zadošča celični porabi kisika. Ta problem smo na osnovi upoštevanja izmerjene snovne bilance kisika uspešno rešili z uvajanjem čistega kisika v bioreaktor. Z grafično predstavitvijo rezultatov smo prikazali možnost kontrole in vodenja procesa. Objava:

– TISU, Matjaž, PAVKO, Aleksander. *Oxygen transfer in a laboratory stirred tank bioreactor during mammalian cell culture cultivation. Acta chim. slov.. [Tiskana izd.], 2010, vol. 57, no. 1, str. 123–128.* [COBISS.SI-ID 33794309].

Biosorpcija svinca na v laboratorijski koloni s strnjenim slojem imobilizirane biomase glive Rhizopus nigricans v peletni obliki: matematični model in eksperiment: V laboratorijski koloni smo proučevali biosorpcijo svinčevih ionov iz vodne raztopine na imobilizirani biomasi glive *Rhizopus nigricans*. Izmerjene prebojne krivulje smo primerjali z izračunanimi s pomočjo matematičnega modela, ki smo ga razvili za simulacijo adsorpcije na peletih mehke glivne biomase. Pri proučevanih pogojih na prebojno krivuljo zelo vplivata poroznost in adsorpcijska kapaciteta biomase. Snovni tok kontrolira upor v filmu zunaj peleta, medtem ko upor znotraj peleta in aksialno disperzijo lahko zanemarimo. V model smo uvedli nov parameter α ki predstavlja delež aktivne biomase in za naš primer znaša $\alpha = 0,7$. Tako smo upoštevali specifične lastnosti biomase in posledično tudi neidealni tok skozi sloj glivnih peletov. Objava:

– KOGEJ, Adela, LIKOZAR, Blaž, PAVKO, Aleksander. *Lead biosorption by self-immobilized Rhizopus nigricans pellets in a laboratory scale packed bed column : mathematical model and experiment. Food technol. biotechnol., 2010, vol. 48, no. 3, str. 344–351.* [COBISS.SI-ID 34326021].

Vpliv aksialnih in radialnih mešal na prenos toplote v industrijskih bioreaktorjih: Študirali smo vpliv aksialnih in radialnih mešal na prenos toplote v industrijskih bioreaktorjih. Raziskave so obravnavale vpliv procesne reologije, ki se je, z ozirom na rast glivine biomase, spreminjala od newtonske do psevdoplastične, na prenos toplote. Uporaba aksialnih mešal v primerjavi z radialnim načinom mešanja, se je izkazala za precej učinkovitejši način mešanja v velikem merilu. Objava:

– MERWE, Jacob D. van der, MINARIK, Martin, BEROVIČ, Marin, HERAKOVIČ, Niko. *Heat transfer in citric acid production with axial and radial flow impellers. Acta Chim. Slov, 2010, vol. 57, no. 1, str. 150–156. http://acta.chem-soc.si/57/57-1-150.pdf.* [COBISS.SI-ID 33809925].

Čiščenje odpadne vode s pritrjeno biomaso v obliki biofilma: Učinkovitost procesa čiščenja odpadne vode s pritrjeno biomaso v obliki biofilma na nosilnih elementih temelji na celotni razpoložljivi površini nosilnega elementa v reaktorju. Specifična površina je tako parameter, ki omogoča primerjavo delovanja procesov čiščenja odpadne vode z uporabo različnih nosilnih elementov. V naši študiji smo določili aktivno specifično površino sferičnih poroznih nosilnih elementov iz polivinil alkohola (PVA gel) podjetja Kuraray (Japonska), katere predhodne študije so pokazale učinkovito naselitev tako heterotrofnih kot avtotrofnih mikroorganizmov. Določitev smo izvedli na osnovi kalibracije napovedi matematičnega modela v GPS-X

(Hydromantis) orodju in empiričnih rezultatov procesa čiščenja v dveh različno vodenih pilotnih sistemih. Objava:

– LEVSTEK, Meta, PLAZL, Igor, ROUSE, Joseph D. *Estimation of the specific surface area for a porous carrier. Acta chim. slov., 2010, 57, 45-51.* [COBISS.SI-ID 33804037].

Čiščenje deponijskih odpadnih vod: Preučevali smo učinkovitost naprednih oksidacijskih procesov (AOPs) za odstranjevanje biološko stabilnih nevarnih organskih onesnaževal iz deponijskih izcednih vod. Primerjali smo možne načine čiščenja deponijskih izcednih vod z različnimi metodami v odvisnosti od fizikalno-kemijskih in ostalih pogojev. Učinkovitost postopkov smo spremljali s kemijskimi analizami in biotesti, ki so zajemali vrednotenje vpliva na več členov ekosistema. To je bila osnova za presojo vpliva na okolje in spremljanja učinkov različnih načinov čiščenja odpadnih vod. Usmerili smo se predvsem v fizikalno-kemijske postopke čiščenja problematičnih odpadnih vod. S kombinacijo različnih fizikalno-kemijskih in bioloških postopkov smo identificirali tudi vire problematičnih komponent v odpadnih vodah in prispevali k optimizaciji obstoječih in razvoju čistejših proizvodnih tehnologij. V sklopu raziskav smo se posvetili tudi razvoju novih kroničnih strupenostnih testov z organizmom *Artemia salina* in razvoju strupenostnih testov z višjimi rastlinami z merjenjem encimskih odzivov. Objave:

– NAKRST, Jana, BISTAN, Mirjana, TIŠLER, Tatjana, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. *Feasibility of Fenton's oxidation for removal of estrogens from aqueous solutions. Acta chim. slov.. [Tiskana izd.], 2010, vol. 57, no. 1, str. 90–99. http://acta.chem-soc.si/57/57-1-090.pdf.* [COBISS.SI-ID 33808389].
– DERCO, Ján, ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana, ALMÁSIOVÁ, Beáta, KASSAI, Angelika. *Pretreatment of landfill leachate by chemical oxidation processes. Chem. zvesti, 2010, vol. 64, no. 2, str. 237–245, doi: 10.2478/s11696-009-0116-5.* [COBISS.SI-ID 33642501].
– COTMAN, Magda, ŽGAJNAR GOTVAJN, Andreja. *Comparison of different physico-chemical methods for the removal of toxicants from landfill leachate. J. hazard. mater.. [Print ed.], 2010, vol. 178, no. 1/3, str. 298–305, doi: 10.1016/j.jhazmat.2010.01.078.* [COBISS.SI-ID 33885701].
– KALČÍKOVÁ, Gabriela, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. *Evaluation of landfill leachate quality with battery of biotests. Acta Environ. Univ. Comen., 2011, vol. 19, suppl. 1, str. 145–150.* [COBISS.SI-ID 34893573].
– ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana, COTMAN, Magda. *Fenton's oxidative treatment of municipal landfill leachate as an alternative to biological process. Desalination. [Print ed.], str. 1–7., doi: 10.1016/j.desal.2011.03.017.* [COBISS.SI-ID 34925829].

DRUGI RELEVANTNI DOSEŽKI

UREDNIŠTVO

– Acta chimica slovenica. Pavko, Aleksander (glavni urednik 2006–, gostujoči urednik 2010). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: = Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]
– Chemical and biochemical engineering quarterly. Plazl, Igor (urednik 2009–). Zagreb: Croatian Society of Chemical Engineers, 1987–. ISSN 0352-9568. [COBISS.SI-ID 49186]
– Kemija u industriji. Plazl, Igor (član uredniškega odbora 2009–). [Print ed.]. Zagreb: Hrvatsko društvo kemijskih inženjera i tehnologa, 1952–. ISSN 0022-9830. http://nippur.irb.hr/hrv/kui. [COBISS.SI-ID 747524]

– Chemical and biochemical engineering quarterly. Žnidaršič Plazl, Polona (članica uredniškega odbora 2009–). Zagreb: Croatian Society of Chemical Engineers, 1987–. ISSN 0352-9568. [COBISS.SI-ID 49186]
– European water management. Zagorc-Končan, Jana (članica uredniškega odbora 1998–). Lavenham: Terence Dalton Publishers, 1998–. ISSN 1461-6971. [COBISS.SI-ID 1607450]

PREDAVANJE NA TUJI UNIVERZI ALI RAZISKOVALNI INSTITUCIJI

– PAVKO, Aleksander. Fungal bioremediation : [École Polytechnique Féderale de Lausanne, EPFL, 18. October 2010]. Lausanne, 2010. [COBISS.SI-ID 34556165]
– ŽGAJNAR GOTVAJN, Andreja. Environmental problems in Slovenia : [Faculty of Chemistry, Brno University of Technology, Brno, February 18, 2010]. 2010; Brno. [COBISS.SI-ID 33741829]
– ŽGAJNAR GOTVAJN, Andreja, JUG, Aleš. Faculty of Chemistry and Chemical Technology : study programmes and research work : [Norwegian University of Science and Technology (NTNU), 25th October 2010]. Trondheim, 2010. [COBISS.SI-ID 34572549]

ORGANIZACIJA MEDNARODNEGA KONGRESA

– International Thematic Conference »Implementation of Microreactor Technology into Biotechnology«, Ljubljana, September 29–30, 2010, ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). IMTB 2010 : [proceedings CD]. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010. 1 optični disk (CD-ROM). ISBN 978-961-6756-20-4. [COBISS.SI-ID 252678656]

BILATERALNI PROJEKTI

– Slovenija – Kitajska: Produkcija farmacevtsko aktivnih spojin *Grifola frondosa* s postopkom gojenja na trdnem in tekočem gojišču. Nosilec: M. Berovič.
– Slovenija – Bolgarija: Mikrobiološke transformacije steroidov v sistemu mikrokanalov. Nosilka: P. Žnidaršič Plazl.
– Slovenija – Portugalska: Implementacija mikrostrukturiranih naprav v procese biotransformacij in bioseparacij. Nosilec: I. Plazl.
– Slovenija – Madžarska: Kompoziti guma/poliuretan/nanopolnilo: Struktura in lastnosti. Nosilka: U. Šebenik.
– Slovenija – Ciper: Pretočnost modelnih telesnih tekočin skozi žile in srčne poti. Nosilka: A. Zupančič Valant.

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA

Mednarodno znanstveno sodelovanje, ki ga financira Nacionalna fundacija za znanost, visoko šolstvo in tehnološki razvoj Republike Hrvaške – raziskovalni projekt: Sinteza ionskih tekočin in biotransformacije s temi topili v mikroreaktorjih. Nosilka: P. Žnidaršič Plazl.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

The programme content covers studies of transport phenomena in heterogeneous reaction-diffusion systems, which include mathematical and physical description of processes at different levels of observation, from molecular to macroscopic, development of nonlinear systems for process description, and tailor-made product development for specific applications, which require detailed knowledge of complex transport mechanisms. This research enables an integrated multidisciplinary systematic approach, the development of fundamental chemical engineering scientific knowledge and its application in the specific areas of chemical engineering. Programme goals have been set up according to the specific branches of chemical engineering,: *chemical process engineering with rheology, polymer engineering, biochemical engineering and environmental engineering.*

CHEMICAL PROCESS ENGINEERING WITH RHEOLOGY

Microtechnology has opened completely new scientific challenges and useful solutions in a broad range of fields, from electronic industry, medical technology, fuel production and processing, biotechnology, chemical industry, environmental protection and process safety. Microstructured devices have demonstrated several advantages in (bio)chemical processes, due to a very large surface-area-to-volume ratio connected with highly effective heat and mass transfer, easier control of process parameters and new production concepts. There are suggestions that there could be benefits for fine chemical/pharmaceutical industries where about 50% of the reactions could be used in a continuous process based mainly on microreactor technology. In this research the microfluids phenomena and reaction-diffusion dynamics of different (bio)chemical processes in microstructured devices were studied and applied in developed integrated lab-on-a-chip systems.

Multiphase systems are integrated in many industrial processes. High level of fundamental knowledge is crucial for a suitable and effective design of a selected device. According to the selected level of control volume it is possible to describe the behaviour of multiphase system through sophisticated numerical solutions of the balances of transport quantities, or through phenomenological models, based on a thorough experimental work and exact observations of the system. In both cases the goal is to predict fluid dynamic behaviour and transport phenomena in the system as a function of given operating conditions. Non-Newtonian liquids are involved in most bio-chemical processes, yet in literature there is still a certain gap in understanding the impacts of such complex liquids on the performance of a multiphase system. In our previous work with bubble column it was clearly shown that the presence of a non-Newtonian liquid with elastic properties causes highly complex hydrodynamic behaviour of the system; instead of time and volume-averaged approach in evaluation of the measured quantities, local time-dependant measurements of the experimental data is needed, which would enable the development of a discrete cell model, or a reliable CFD model approach.

Concentration of the product in water solution is one of the important steps in downstream process technologies. Evaporation is one of the possibilities, where low pressure conditions need to be taken into account in case of a thermally unstable solute. Evaporation has been often successfully replaced by membrane separation technologies due to lower investment and operating costs as well as low temperature operating conditions. In the last decade, the research and applications of product concentration in organic solvents with nanofiltration have increased.

Several models, which take into account porous structure of the membrane, molecule diffusion in the membrane, resistances in series, as well as surface tension of the membrane and solvent, have been developed to describe the organic solvent flux and solute rejection. By the selection of industrial solvents and solutes and by measuring the solvent flux and solute rejection the research is applicative. However, by the explanation of solvent and solute transport through membrane and solute separation with the existing models, or newly developed model, the basic nature of the research will be given. The research focuses on laminar film on the concentrate side of the membrane and interactions between membrane, solute and solvent. The goal is to assess the membrane area and make economical comparison between nanofiltration and evaporation for a selected system.

Rheology and applications – knowledge about flow behaviour of rheologicaly complex fluids – is essential for understanding the peculiarity of technological process in which fluids function as process fluids or as final products. Real fluids, such as heterogeneous systems, are non-Newtonian since they exhibit various responses on the action of shear forces and on shear flow. This is due to complex internal structures present in liquid material. The internal liquid structure of polymer material can be considered as a configuration of polymer molecules. The responses on shear flow depend on molecular interactions and on the combination of attractive and repulsive interactions between the components present in heterogeneous liquids. In the research study, rheological properties of heterogeneous polymer melts will be examined in order to determine key factors for the composition, which tailor mechanical properties of polymer materials. Rheological models for describing shear dependent behaviour (constitutive equations) of heterogeneous polymer systems of different compositions will be determined from experimental data. These models will be used to determine appropriate formulation of polymer material with target mechanical properties and to examine transport parameters of microstructures.

The characterization of blood flow is important for understanding the function of cardiovascular system under normal and diseased conditions. For a complete description of thermodynamics phenomena, it is essential to define the appropriate viscous model, which takes into account the low and high shear rate behaviour of blood. During the course of the project some rheological models for describing shear dependent properties of blood, physiological and cardioplegic solutions and their temperature dependence will be determined on the basis of experimental rheological data. Rheological properties of blood will be compared with some model body fluids of different composition (volume expanders and other polysaccharides) in order to determine the main factors that influence their flow properties and the dependence on temperature. Proper constitutive equations with temperature-dependent material parameters will be proposed for the biological fluids investigated based on experimental data, and will be tested in models of two- and three- dimensional geometries. These results may guide the improvement of certain physiological and cardioplegic solutions and their optimal use in practice. The numerical simulation of the flow of these fluids in realistic geometries, such as arteries and other blood vessels, at different temperatures will provide useful information for heart surgery.

POLYMER ENGINEERING

Micro-encapsulation is a process in which tiny particles or droplets are surrounded by a coating to give small capsules with many useful properties. The material inside the microcapsule is referred to as the core, internal phase, or a fill, whereas the wall is sometimes called a shell, coating, or membrane. The reasons for microencapsulation are countless. In some cases, the

core must be isolated from its surroundings, as in isolating vitamins from the deteriorating effects of oxygen, retarding evaporation of a volatile core, improving the handling properties of a sticky material, or isolating a reactive core from chemical attack. In other cases, the objective is not to isolate the core completely but rather to control the rate at which the core leaves the microcapsule, as in the controlled release of drugs or pesticides. The problem may be simple, i.e. masking the taste or odour of the core, or complex, i.e. increasing the selectivity of the adsorption or extraction process. The goal of the research program is to develop a method for micro-encapsulation of different core substances in a polymeric shell. Different polymers, such as melamine-formaldehyde resin, will be used as shell material. The polymerization and curing processes by which the shell is formed are studied. The application properties of microcapsules are described also by studying the mass release from the core through the shell into the environment.

Pressure sensitive adhesives (PSA) are defined as materials, which in dry form are aggressive and permanently tacky at room temperature and firmly adhere to a variety of dissimilar surfaces upon mere contact, without the need of more than finger pressure. PSAs are used for numerous products in many different ways. Acrylic polymers are one of the most widely used materials for the production of pressure sensitive adhesives. The PSAs can be segmented by type of technology used to convert the adhesive into its final form: solvent-based, water-based, hot melt, UV cured, etc. The first part of the research is focused on the suspension polymerization by which microspheric water-based PSA adhesives are obtained. The main goal is to develop a method and a process by which tailor-made product can be made. The research work includes nanocomposite PSA adhesives synthesis and characterization. Another goal of the research is to develop a new, commercially suitable RT UV PSA acrylic adhesive, which may be applied on the substrate and cross linked by UV light at room temperature. Heat transfer during bulk polymerization of acrylic monomers is being studied as well.

The synthesis of polysiloxane emulsions by anionic emulsion polymerization with ring opening reaction is being studied. The goal is to investigate the effect of composition and reaction parameters on emulsions end properties. At the same time complex mechanisms of the synthesis will be proposed.

The kinetics of synthesis and cross linking of different formaldehyde resins is being studied to optimize the production process and develop a technology of melamine foam production.

The kinetics of vulcanization process and heat transfer during vulcanization process for selected rubber blends have been studied. The processes were described by mathematical modelling. New rubber nanocomposites were prepared and their viscoelastic behaviour was determined and modelled on a wide range of temperatures and frequencies. Other relevant nanocomposite properties were determined by different characterization methods. The dependence of the properties on the composition and structure were studied as well.

BIOCHEMICAL ENGINEERING

Biotransformations and biodegradations of chemical compounds of natural and synthetic origin are applied in several chemical, pharmaceutical and food industries, particularly in the processes of fine chemicals and environmental protection. Among priority goals is the design of processes employing immobilized enzymes or whole cells, which can be used repeatedly for as long as they remain active, by minimizing costs and enabling economically feasible operation in a continuous mode. Furthermore, integrated process operation with chemical operations and downstream processes would enable highly efficient and environmentally sustainable produc-

tion. Integration of biocatalytic processes with microreactor technology is of a great potential in this field. In recent years, a successful application of enzymatic microreactors has been reported, mainly in chemical analysis and kinetic studies. Within the research programme, the development of a continuous process of selected biotransformations in a microreactor with immobilized cells/enzymes and with integrated product separation is envisaged. Microreactor technology will further gain from the useful symbiosis between nanotechnology and ionic liquids which have recently received an increased attention as "green" solvents for organic synthesis in general and catalytic processes in particular. Recently, the use of ionic liquids as reaction media has been extended to enzymatic catalysis and whole cell biotransformations. However, their use in industrial processes is restricted due to high market prices, so the development of the processes with these solvents at a microscale level is suggested as a promising alternative.

The influence of transport phenomena of rheological changeable cultivation media in heterogeneous reaction-diffusive system and its influence on basidiomyces biosynthesis of pharmaceutically active compounds with antitumor, anticancer and imunostimulatory activities, as well its influence on technology of production, isolation and purification of the products and their *in-vitro* testing has been studied.

ENVIRONMENTAL ENGINEERING

Applied biocatalysis in the field of bioremediation is a relatively young science yet gaining significance in environmental engineering. The problems of industrial organic waste streams can be solved with enzymes and microbes in environmentally friendly way. The interest to use white rot fungi for the bioremediation purposes has substantially increased in the last decade. These microorganisms degrade organic aromatic pollutants with lignin degrading enzymes, e.g. manganese peroxidase, lignin peroxidase and laccase, especially if they grow immobilized on a proper solid support. The extracellular, as well as the intracellular enzyme activities can be induced by proper selection of a liquid substrate composition and support material as well as selection of growth conditions. On the basis of previous investigations the rotating discs reactor seems to be a promising reactor type. In the proposed research, the effect of liquid substrate composition and solid support material on specific enzyme activities and degradation rates for selected organic pollutant – industrial organic dyes is currently being investigated. The main goal is to acquire new knowledge about the use of fungi and enzymes in solving problems of industrial organic waste effluents with bioremediation by environmentally friendly technology. From the economic perspective, the bioremediation under non-sterile conditions is cheaper; therefore the comparison of the process efficiency under sterile and non-sterile conditions is interesting. By experiments with real samples the industrial applicability is being evaluated.

RESEARCH TOPICS

Chemical process engineering with rheology:

- Microreactor technology
- Desorption of metals from soil in continuous system
- Experimental study of hydrodynamics and kinetic/adsorption parameters of expanded-bed column
- Isolation af active pharmaceutical agents
- Rheologicaly complex fluids

Polymer engineering

- Microencapsulation research
- Synthesis, characterization and synthesis process optimization of acrylic adhesives
- Synthesis, characterization and synthesis process optimization of nanocomposite materials
- Synthesis, characterization and synthesis process optimization of polysiloxane emulsions
- Synthesis, characterization and optimization of the synthesis process of formaldehyde resins
- Research and development of a technology for the production of melamine foams
- Kinetic investigations during vulcanization process for different rubber blends and modelling
- Heat transfer investigations during vulcanization process for different rubber blends and modelling
- Testing of rubber and rubber composites

Bioengineering and biotechnology

- Continuous biotransformation of progesterone
- Steroid extraction in a microchannel system
- Biocatalytic reactions in a microchannel system
- Enzyme catalyzed synthesis of isoamyl acetate in a microreactor
- Optimization of submerged and solid state cultivation of pharmaceutically active fungal biomass
- Biosynthesis of extra and intracellular fungal polysaccharides on secondary wastes generated by wood and agricultural industries
- Cultivation of *Grifola frondosa* fungal fruit bodies on secondary wastes generated by wood and agricultural industry
- Isolation and purification of extra and intracellular fungal polysaccharides
- In-vitro testing of immunostimulatory activities of isolates by induction of cytokines in human peripherial mononuclear blood cells (PBMC)

Environmental engineering

- Bioremediation research
- Nitrification in the moving-bed biofilm process
- Biological and physico-chemical methods of wastwater treatment
- Advanced oxidation processes for toxic organic pollutants removal from wastewaters
- New chronic test with *Artemia slina*
- Toxicity tests with higher plants on enzymatic level
- Environmental impact of ionic liquids as solvents

SCIENTIFIC ACHIEVEMENTS

Microtechnology: Microtechnology has opened completely new scientific challenges and useful solutions in a broad range of areas, from electronic industry, medical technology, fuel production and processing, to biotechnology, chemical industry, environmental protection and process safety. Microstructured devices have demonstrated several advantages in (bio)chemical processes, due to the very large surface-area-to-volume ratio connected with very effective

heat and mass transfer, easier control of process parameters and new production concepts. There are suggestions that in fine chemical/pharmaceutical industry about 50% of reactions could benefit from a continuous process based mainly on microreactor technology. Within our research, various homogeneous and heterogeneous systems were studied within microreactors and compared with literature data for processes in classical reactors. The achievements have been published in:

– PLAZL, Igor, LAKNER, Mitja. *Modeling and finite difference numerical analysis of reaction-diffusion dynamics in a microreactor. Acta chim. slov.. [Printed ed.], 2010, Vol. 57, No. 1, p.p. 100–109. http://acta.chem-soc.si/57/57-1-100.pdf.* [COBISS.SI-ID 33804805].

Desorption of metals from soil in continuous system: Physical processes controlling the desorption of some elements (B, Cd, Co, Mn, Ni, and Sr) from soils in a continuous leaching system representing a human stomach have been investigated by fitting experimental leaching data to a mathematical particle diffusion model. Soil samples (50 mg) from Cornwall, UK, were intimately contacted with artificial gastric solution at various flow rates for up to approx. 4 h, followed by the analysis of the collected fractions with inductively coupled plasma mass spectrometry (ICP-MS). The leaching profiles of the various elements were fitted to a mathematical model and incorporated two mass transfer processes (liquid film diffusion and apparent solid phase diffusion). A system of partial differential equations was solved numerically by finite difference discretization of the computational domain. Publication:

– BEESTON, Michael Philip, POHAR, Andrej, ELTEREN, Johannes Teun van, PLAZL, Igor, ŠLEJKOVEC, Zdenka, VEBER, Marjan, GLASS, Hylke J. *Assessment of physical leaching processes of some elements in soil upon ingestion by continuous leaching and modeling. Environ. sci. technol.. [Print ed.], 2010, Vol. 44, issue 16, p.p. 6242–6248, doi: 10.1021/es1006725.* [COBISS.SI-ID 4448538].

Rheologicaly complex fluids: Blood rheology and hemodynamics: The characterization of blood flow is important for understanding the function of the cardiovascular system under normal and diseased conditions. On the basis of experimental rheological data the rheological models for describing shear dependent properties of blood, cardioplegic solutions (volume expanders) and their mixtures as well as their temperature-dependence were determined. Rheological properties of blood (taken from different donors) were compared with blood mixtures with volume expanders of different composition in order to determine the main factors that influence their flow properties and its dependence on temperature.

Proper constitutive equations with temperature-dependent material parameters were proposed for investigated blood mixtures based on the above measurements which were tested in models of three- dimensional geometries. The research on hemodynamics has been done in collaboration with colleagues from Cyprus (bilateral project). They developed a high fidelity transient numerical simulation of blood using appropriate constitutive equations in coronary arteries and other blood vessels at different temperature regimes. These results may guide the improvement of certain physiological and cardioplegic solutions and their optimal use in practice. The numerical simulation of the flow of these fluids in realistic geometries, such as arteries and other blood vessels, at different temperatures will provide useful information for heart surgery. The research work was published in:

– ZUPANČIČ-VALANT, Andreja, ŽIBERNA, Lovro, PAPAHARILAOU, Yannis, ANAYIOTOS, Andreas, GEORGIOU, Georgios C. *The influence of temperature on rheological properties of blood mixtures with different volume expanders: implications in numerical arterial hemodynamics simulations. Rheol. Acta, doi: 10.1007/s00397-010-0518-x.* [COBISS.SI-ID 34768133].

The investigation of rubber modified bitumen as a binder for production of asphalt mixtures: The rheological properties of rubber modified bitumen were investigated. Publication:

– LUKAČ, Bojana, ZUPANČIČ-VALANT, Andreja. *Raziskovanje obnašanja gumibitumna kot veziva za proizvodnjo gumiranih asfaltnih zmesi = The investigation of rubber modified bitumen as a binder for production of asphalt mixtures. Gradb. vestn., 2010, Vol. 59, No. 11, p.p. 261–268.* [COBISS.SI-ID 34588933].

Microencapsulation: The main objective was to investigate the composition of microcapsules and the degree of cure of melamine–formaldehyde (MF) resin, which formed a shell of microcapsules, by the use of differential dynamic calorimetry (DSC). For this purpose, decane was chosen as a core material. The microencapsulation of decane with MF resin was carried out at different temperatures and pH values. The temperature and the pH value were kept constant during the process. The composition of the microcapsules and the degree of curing of the shell material were studied during and after the microencapsulation process. DSC analysis, in combination with scanning electron microscopy analysis, proved to be an effective tool for the investigation of the microencapsulation process with MF resin. Publication:

– ALIČ, Branko, ŠEBENIK, Urška, KRAJNC, Matjaž. *Differential scanning calorimetric examination of melamine-formaldehyde microcapsules containing decane. J. appl. polym. sci., 2011, Vol. 119, No. 6, p.p. 3687–3695, doi: 10.1002/app.33077.* [COBISS.SI-ID 34469637].

Synthesis, characterization and optimization of the synthesis process of acrylic adhesives: The synthesis and characterization of UV crosslinkable acrylic pressure sensitive adhesives was studied. Different amounts of unsaturated photoinitiator 4-acryloyloxy benzophenone (4-ABF) were added in t-butyl acrylate/2-ethylhexyl acrylate monomer mixture and then polymerized, using the suspension polymerization technique. The adhesive suspension was coated on a pilot coating machine, dried by IR and subsequently crosslinked under UV light. Upon absorption of UV light,the copolymerized 4-ABF photoinitiator produced reactive radicals which are capable of initiating a rapid chain reaction with the neighboring C–H positions of polymer side chains, which leads to the formation of crosslinked polymer structures. UV crosslinking process was monitored by ATR-FTIR spectroscopic technique. Adhesion properties of the synthesized materials were determined using standard measurements of tack, peel and shear strength. Publication:

– KAJTNA, Jernej, KRAJNC, Matjaž. *UV crosslinkable microsphere pressure sensitive adhesives : influence on adhesive properties. Int. j. adhes. adhes.. [Print ed.], 2011, Vol. 31, No. 1, p.p. 29–35, doi: 10.1016/j.ijadhadh.2010.09.004.* [COBISS.SI-ID 34530309].

Synthesis, characterization and optimization of the synthesis process of polysiloxane emulsions: Batch anionic ring-opening polymerization of octamethylcyclotetrasiloxane in emulsion using nonionic and cationic emulsifiers was studied. Effects of emulsifier concentration, nonionic/cationic emulsifier ratio and cationic emulsifier/initiator (KOH) ratio on the kinetics, average particle size and distribution and on the average molecular weight and distribution were investigated and discussed. The transport of monomer from monomer droplets towards empty micelles was confirmed by monomer droplets and empty micelles disappearance and by the formation of smaller particles. The transport of monomer from monomer droplets towards polymer particles was not confirmed, since the average polymer particle size did not increase during polymerization. It was proposed that at lower conversions, monomer diffuses from polymer particle interior to particle surface, while at higher conversions, the monomer diffuses from larger to smaller polymer particles. Emulsifier concentration, nonionic/cationic emulsifier ratio and cationic emulsifier/KOH ratio have an evident effect on the kinetics and

on the average molecular weight, thus demonstrating that cationic emulsifier participates to the initiation reaction. Publication:

– MOHORIČ, Ines, ŠEBENIK, Urška. *Anionic ring-opening polymerization of octamethylcyclotetrasiloxane in emulsion above critical micelle concentration. Polymer (Guildf.). [Print ed.], 2011, Vol. 52, Bo. 5, p.p. 1234–1240, doi: 10.1016/j.polymer.2011.01.025.* [COBISS.SI-ID 34739717].

Microreactor technology in biochemical engineering: The enzymatic oxidation of cholesterol to 4-cholesten-3-one performed within microchannels by cholesterol oxidase, was studied in a two phase system, comprising an organic phase as a substrate and product pool, and an aqueous phase with dissolved enzyme. A mathematical model, comprising double substrate Michaelis-Menten kinetics and the velocity profile of two immiscible fluids, was developed in order to describe and predict the process of cholesterol oxidation. In a Y shape microreactor geometry, roughly up to 70% conversion of cholesterol was achieved at residence times below 1 min. A suitable adjustment of the fluid flow rates allowed for phase separation at the Y-shaped exit from the microreactor and thereby enabled in situ product separation from the aqueous phase containing the enzyme. *Saccharomyces cerevisiae* was successfully immobilized on the inner wall surface of channels of submillimeter diameter,which can be further used for the development of a highly productive continuous biotransformation process within a microfluidic device. This is the first report on cell immobilization onto PTFE, FEP and PFA surface, which enables to develop a microfluidic device with surface bound biocatalyst from low-cost and disposable materials. Furthermore, an integrated approach for the improvement of progesterone 11α-hydroxylation by *Rhizopus nigricans*, was accomplished. Several issues have been addressed in order to increase process productivity, including biocatalyst immobilization, improvements in the solubility of the lipophilic substrate, setting-up of continuous reaction process and easing downstream processing. In order to develop an integrated biotransformation process, a continuous two-liquid phase extraction within microchannel device has been set up, where very efficient steroid extraction was achieved within a few seconds. Publications:

– MARQUES, M. P. C., FERNANDES, P., CABRAL, Joaquim M. S., ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. *On the feasibility of in-situ steroid biotransformation and product recovery in microchannels. Chem. Eng. J., 2010, 160, 708–714, doi: 10.1016/j.cej.2010.03.056.* [COBISS.SI-ID 33911813].
– STOJKOVIČ, Gorazd, ŽNIDARŠIČ PLAZL, Polona. *Immobilization of yeast cells within microchannels of different materials. Acta chim. slov., 2010, 57, 144–149. http://acta.chem-soc.si/57/57-1-144.pdf.* [COBISS.SI-ID 33807877].
– ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. *Development of a continuous steroid biotransformation process and product extraction within microchannel system. Catal. Today, 2010, 157, 315–320, doi: 10.1016/j.cattod.2010.01.042.* [COBISS.SI-ID 33681925].
– STOJKOVIČ, Gorazd, PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. *L-Malic acid production within a microreactor with surface immobilised fumarase. Microfluid. nanofluid., doi: 10.1007/s10404-010-0696-y.* [COBISS.SI-ID 34517509].

Oxidation of coniferyl alcohol catalyzed by commercial laccase and crude laccase: Oxidation of coniferyl alcohol catalyzed by commercial laccase and crude laccase produced during the submerged cultivation of *Trametes versicolor* in a medium containing waste from paper industry was investigated. Mathematical model of batch process, which includes double-substrate Michaelis-Menten kinetics with oxygen as the second substrate and mass balances, has been developed and validated in experiments with or without additional aeration. 100%

conversions of up to 0.8 mM of coniferyl alcohol in batch experiment due to high operational stability of enzymes was realized with both laccases. Publication:

– TIŠMA, Marina, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor, VASIĆ-RAČKI, Đurđa, ZELIĆ, Bruno. *Oxidation of coniferyl alcohol catalyzed by laccases from Trametes versicolor. Acta chim. slov. 2010, 57, 110–117. http://acta.chem-soc.si/57/57-1-110.pdf.* [COBISS.SI-ID 33807109].

Oxygen transfer in a laboratory stirred tank bioreactor during mammalian cell culture cultivation: The influence of stirrer speed and power consumption on the volumetric mass transfer coefficient was studied in a 5 liter stirred tank bioreactor during cultivation of a recombinant CHO cell line, which requires low aeration and mixing intensity. Under these conditions and at high cell concentrations, oxygen mass transfer rates were not sufficient for a given oxygen consumption. This problem was successfully solved on the basis of measured oxygen mass balance by introducing pure oxygen into the bioreactor. A graphic presentation of the results showed the possibilities of the process regulation and control. Publication:

– TISU, Matjaž, PAVKO, Aleksander. *Oxygen transfer in a laboratory stirred tank bioreactor during mammalian cell culture cultivation. Acta chim. slov.. [Tiskana izd.], 2010, Vol. 57, No. 1, p.p. 123–128.* [COBISS.SI-ID 33794309].

Lead biosorption by self-immobilized Rhizopus nigricans pellets in a laboratory scale packed bed column: mathematical model and experiment: The biosorption of lead ions from aqueous solution on a self-immobilized *Rhizopus nigricans* biomass was studied in a laboratory column. Experimental breakthrough curves were compared to those predicted by a mathematical model, which was developed to simulate a packed bed biosorption process by a soft, self-immobilized fungal biosorbent. In the range of experimental conditions, the biomass characteristics, such as pellet porosity and biosorption capacity, substantially affected the predicted response curve. The external film resistance controls the mass transfer, while the intra-pellet mass transfer resistance and the effect of axial dispersion, can be neglected. A new parameter α, the fraction of active biomass, with an average value of $\alpha = 0.7$, was introduced to take into account the specific biomass characteristics, and the observed non-ideal liquid flow through the bed of fungal pellets. Publication:

– KOGEJ, Adela, LIKOZAR, Blaž, PAVKO, Aleksander. *Lead biosorption by self-immobilized Rhizopus nigricans pellets in a laboratory scale packed bed column : mathematical model and experiment. Food technol. biotechnol., 2010, Vol. 48, No. 3, p.p. 344–351.* [COBISS.SI-ID 34326021].

Heat transfer in citric acid production with axial and radial flow impellers: The focus of the fermentation study was directed towards obtaining information on broth rheology, heat transfer aspects and considerations. Broth rheology was found to deviate from Newtonian behavior with increasing biomass concentration. Using axial flow impellers, rather than radial flow producing Rushton turbines, significantly improved heat transfer in this study. Publication:

– MERWE, Jacob D. van der, MINARIK, Martin, BEROVIČ, Marin, HERAKOVIČ, Niko. *Heat transfer in citric acid production with axial and radial flow impellers. Acta Chim. Slov, 2010, Vol. 57, No. 1, p.p. 150–156. http://acta.chem-soc.si/57/57-1-150.pdf.* [COBISS.SI-ID 33809925].

Wastewater treatment in the moving-bed biofilm reactor: In biofilm systems, treatment performance is primarily dependent upon the available biofilm growth surface area in the reactor. Thus, specific surface area is a parameter which allows for making comparisons between

different carrier technologies used for wastewater treatment. In this study, we estimated the effective surface area for a spherical, porous polyvinyl alcoho1l (PVA) gel carrier (Kuraray) that has previously demonstrated effectiveness for retention of autotrophic and heterotrophic biomass. This was accomplished by applying the GPS-X modeling tool (Hydromantis) to a comparative analysis of two moving-bed biofilm reactor (MBBR) systems. Publication:

– LEVSTEK, Meta, PLAZL, Igor, ROUSE, Joseph D. *Estimation of the specific surface area for a porous carrier. Acta chim. slov., 2010, 57, 45–51.* [COBISS.SI-ID 33804037].

Wastewater treatment – Landfill leachate treatment: Different treatment procedures have been studied using different methods under various physico-chemical and other conditions. Treatment efficiency was assessed by chemical analyses and different biotests to monitor impact to various organisms. The research work was focused on physico-chemical treatment methods of complex persistent wastewaters, landfill leachates mainly. Combination of different physico-chemical and biological processes was used to identify the sources of toxic compounds in wastewaters. This leads to optimization of industrial processes and implementation of greener technologies. Publications:

– NAKRST, Jana, BISTAN, Mirjana, TIŠLER, Tatjana, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. *Feasibility of Fenton's oxidation for removal of estrogens from aqueous solutions. Acta chim. slov.. [Printed ed..], 2010, Vol. 57, No. 1, p.p. 90–99. http://acta.chem-soc.si/57/57-1-090.pdf.* [COBISS.SI-ID 33808389].
– DERCO, Ján, ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana, ALMÁSIOVÁ, Beáta, KASSAI, Angelika. *Pretreatment of landfill leachate by chemical oxidation processes. Chem. zvesti, 2010, Vol. 64, No. 2, p.p. 237–245, doi: 10.2478/s11696-009-0116-5.* [COBISS.SI-ID 33642501].
– COTMAN, Magda, ŽGAJNAR GOTVAJN, Andreja. *Comparison of different physico-chemical methods for the removal of toxicants from landfill leachate. J. hazard. mater.. [Print ed.], 2010, Vol. 178, No. 1/3, p.p. 298–305, doi: 10.1016/j.jhazmat.2010.01.078.* [COBISS.SI-ID 33885701].
– KALČÍKOVÁ, Gabriela, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. *Evaluation of landfill leachate quality with battery of biotests. Acta Environ. Univ. Comen., 2011, Vol. 19, suppl. 1, p.p. 145–150.* [COBISS.SI-ID 34893573].
– ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana, COTMAN, Magda. *Fenton's oxidative treatment of municipal landfill leachate as an alternative to biological process. Desalination. [Print ed.], p.p. 1–7., doi: 10.1016/j.desal.2011.03.017.* [COBISS.SI-ID 34925829].

OTHER RELEVANT ACHIEVEMENTS

EDITORIAL WORK

– Acta chimica slovenica. Pavko, Aleksander (Editor-in-Chief 2006–, Guest editor 2010). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: = Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]
– Chemical and biochemical engineering quarterly. Plazl, Igor (Editor 2009–). Zagreb: Croatian Society of Chemical Engineers, 1987–. ISSN 0352-9568. [COBISS.SI-ID 49186]
– Kemija u industriji. Plazl, Igor (Editorial board member 2009–). [Print ed.]. Zagreb: Hrvatsko društvo kemijskih inženjera i tehnologa, 1952–. ISSN 0022-9830. http://nippur.irb.hr/hrv/kui. [COBISS.SI-ID 747524]

– Chemical and biochemical engineering quarterly. Žnidaršič Plazl, Polona (Editorial board member 2009–). Zagreb: Croatian Society of Chemical Engineers, 1987–. ISSN 0352-9568. [COBISS.SI-ID 49186]
– European water management. Zagorc-Končan, Jana (Editorial board member 1998–). Lavenham: Terence Dalton Publishers, 1998–. ISSN 1461-6971. [COBISS.SI-ID 1607450]

LECTURES AT FOREIGN UNIVERSITIES OR RESEARCH INSTITUTIONS

– PAVKO, Aleksander. Fungal bioremediation : [École Polytechnique Féderale de Lausanne, EPFL, 18. October 2010]. Lausanne, 2010. [COBISS.SI-ID 34556165]
– ŽGAJNAR GOTVAJN, Andreja. Environmental problems in Slovenia : [Faculty of Chemistry, Brno University of Technology, Brno, February 18, 2010]. 2010; Brno. [COBISS.SI-ID 33741829]
– ŽGAJNAR GOTVAJN, Andreja, JUG, Aleš. Faculty of Chemistry and Chemical Technology : study programmes and research work : [Norwegian University of Science and Technology (NTNU), 25th October 2010]. Trondheim, 2010. [COBISS.SI-ID 34572549]

ORGANISATION OF INTERNATIONAL CONFERENCE

– International Thematic Conference “Implementation of Microreactor Technology into Biotechnology”, Ljubljana, September 29–30, 2010, ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). IMTB 2010 : [proceedings CD]. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010. 1 optični disk (CD-ROM). ISBN 978-961-6756-20-4. [COBISS.SI-ID 252678656]

BILATERAL PROJECTS

– Slovenia – China: Production of Pharmaceutically Active Compounds from *Grifola Frondosa* by Solid State and Submerged Cultivation. Principal researcher: M. Berovič.
– Slovenia – Bulgaria: Microbial Transformations of Steroids within a Microchannel System. Principal researcher: P. Žnidaršič Plazl.
– Slovenia – Portugal: Implementation of Microstructured Devices in Biotransformation and Bioseparation Processes. Principal researcher: I. Plazl.
– Slovenia – Hungary: Rubber/Polyurethane/Nanofiller Systems: Structure and Properties. Principal researcher: U. Šebenik.
– Slovenia – Cyprus: Influence of Volume Expanders on Fluidity of Blood Through Arteries and Other Blood Vessels. Principal researcher: A. Zupančič-Valant.

OTHER FORMS OF INTERNATIONAL COOPERATION

International Scientific Cooperation, sponsored by the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia – Research Project 2009–2010: Synthesis of Ionic Liquids and Biotransformations with these Solvents in Microreactors (Principal researcher: Polona Žnidaršič Plazl).

SEPARACIJSKI PROCESI TOPLOGREDNIH PLINOV ZA TRAJNOSTNI RAZVOJ

SEPARATION PROCESSES OF GREENHOUSE GASES FOR SUSTAINABLE DEVELOPMENT

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P2–0346

VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

prof. dr. Janvit Golob

SODELAVCI PROGRAMSKE SKUPINE / RESEARCH PROGRAMME STAFF

Raziskovalci / Researchers
prof. dr. Janvit Golob
doc. dr. Blaž Likozar
doc. dr. Dušan Klinar
dr. Sergej Knez
dr. Aleksandra Pivec
dr. Klavdija Rižnar

Mladi raziskovalci / Young Researchers
Maja Šoštarič
Franci Malin
Miha Narobe

Sodelujoče institucije / Participating Institutions
Znanstveno-raziskovalno središče Bistra Ptuj

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

TEHNOLOGIJA PRODUKCIJE LIPIDOV Z ALGO *CHLORELLA VULGARIS* V RAZLIČNIH MEDIJIH Z VGRADITVIJO OGLJIKOVEGA DIOKSIDA IZ DIMNIH PLINOV V BIOMASO

Varovanje okolja in izčrpanost zalog surove nafte postajata najpomembnejša izziva s katerima se sooča naftna industrija in posledično ves svet. Izgorevanje fosilnih goriv je najpoglavitnejši vir toplogrednih plinov, odgovornih za globalno segrevanje. Da bi preprečili ali vsaj za nekaj časa prestavili neizogibno približajočo se naftno krizo in dramatično spreminjanje podnebja, so nujno potrebne obnovljive, ogljično nevtralne in ekonomsko dosegljive alternative fosilnim gorivom. Majhen delež tekočih goriv za uporabo v prometu dandanes že predstavljajo goriva pridobljena iz oljnic, medtem ko mikrobna fotosinteza še zdaleč ni raziskana in do nedavnega sploh ni bila predmet raziskav za namen pridobivanja goriv iz mikroorganizmov.

Danes mikroalge, kot surovina za pridobivanje biogoriv, predstavljajo velik izziv številnim znanstvenikom in raziskovalcem po vsem svetu. Mikroalge so hitro rastoči, enocelični ali enostavni večcelični mikroorganizmi, ki v teku procesa fotosinteze fiksirajo ogljikov dioksid (CO_2) in tvorijo energijo v obliki biomase. Algna biomasa se lahko na različne načine uporabi za proizvodnjo energije, in sicer iz algnih lipidov proizvajajo biodizel, med procesom anaerobne digestije algne biomase nastaja metan, s fermentacijo ostankov algne biomase po ekstrakciji lipidov pridobivajo bioetanol, v zadnjem času pa iz alg proizvajajo tudi vodik.

Namen raziskovalnega dela je bil ugotoviti, ali je mikroalga *Chlorella vulgaris* primerna surovina za produkcijo lipidov. Za ta namen je bilo potrebno določiti optimalne pogoje za pridobitev čim večje količine algne biomase, ki bo obenem imela čim večjo vsebnost lipidov.

Raziskali smo različne rastne medije, tako da smo vzporedno z rastjo algne biomase spremljali tudi porabo hranil. Primerjali smo izkoristke različnih ekstrakcijskih metod in v dobljenih ekstraktih analizirali sestavo lipidov.

Ta raziskava je namenjena obvladovanju znanj za zajemanje ogljikovega dioksida iz industrijskih in energetskih procesov in/ali ozračja v smislu pridobivanja energetsko bogatejše biomase.

RAZISKAVE INDUSTRIJSKIH PROCESOV Z NAMENOM EKOLOŠKE IN ENERGETSKE OPTIMIZACIJE

V skladu s programsko zasnovo zniževanja ogljikovega dioksida v ozračju in razvoja znanj za minimizacijo emisij ogljikovega dioksida smo obravnavali različne tehnološke probleme in pridobili rezultate, ki vodijo k boljšim tehnološkim rešitvam obravnavanih procesov, konkretno smo preučevali zapiranje krogotokov v papirni industriji, tehnologijo proizvodnje biodizla in preventivo pri požarih.

RAZISKAVE NA PODROČJU INŽENIRSTVA OKOLJU PRIJAZNIH PROIZVODOV

Značilnost tega dela programskega sklopa so raziskave za razvoj produktov z višjo dodano vrednostjo. Tovrstne raziskave zahtevajo znanja o sintezi, analitiki, separacijskih tehnikah, kinetiki procesa in ostala potrebna znanja z namenom obvladovanja, modeliranja in optimizacije časa

procesa glede na parametrično občutljivost in prenosa dosežkov v laboratoriju v pilotne dimenzije. Nadaljujemo s prenosom tehnologije oborjenih kalcijevih karbonatov v proizvodnjo.

OSREDNJE TEME PROGRAMA

Tehnologija produkcije lipidov z algo Chlorella vulgaris v različnih medijih z vgraditvijo ogljikovega dioksida iz dimnih plinov v biomaso

– zniževanje CO_2 v dimnih plinih
– pridobivanje lipidov s pomočjo *Chlorelle vulgaris*
– optimizacija procesnih pogojev
– modeliranje procesa
– povečevanje procesa in prenos iz laboratorija na pilotni nivo

Raziskave industrijskih procesov z namenom ekološke in energetske optimizacije

– obravnavanje kritičnih faz procesa
– zniževanje specifične porabe energije na enoto produkta
– zniževanje specifičnih emisij CO_2 na enoto produkta
– zniževanje proizvodnih stroškov enote produkta
– zviševanje dodane vrednosti produktov

Raziskave na področju inženirstva okolju prijaznih proizvodov

– zasnova produkta v laboratorijskih dimenzijah
– optimizacija procesnih pogojev za pridobitev produkta
– modeliranje procesa za pridobitev produkta
– prenos dosežkov iz laboratorija na pilotni nivo
– ekonomsko vrednotenje smiselnosti tehnološkega procesa

ZNANSTVENI DOSEŽKI

RAZISKAVE INDUSTRIJSKIH PROCESOV Z NAMENOM EKOLOŠKE IN ENERGETSKE OPTIMIZACIJE

Publikacije:

– Šrekl J., Golob J.: New approach to calculate the probability of ignition, Journal of loss prevention in the process industries, Vol. 24, No. 3 (2011), strani 288–291.
– Šrekl J., Golob J.: Impact of the buildings areas on the fire incidence, Acta chimica slovenica, Vol. 57, No. 1 (2010), strani 118–122.

RAZISKAVE NA PODROČJU INŽENIRSTVA OKOLJU PRIJAZNIH PROIZVODOV

Publikacije:

– Klofutar B., Golob J., Likozar B., Klofutar C., Žagar E., Poljanšek I.: The transesterification of rapeseed and waste sunflower oils : mass-transfer and kinetics in a laboratory batch reactor and in an industrial-scale reactor/separator setup, Bioresource technology, Vol. 101, No. 10 (2010), strani 3333–3344.

DRUGI RELEVANTNI DOSEŽKI

– Golob J.: Kaj lahko pričakujemo od centrov odličnosti?, Zbornik-Državni svet Republike Slovenije, Novo mesto, 2010. stran 7.

TEHNOLOGIJA PRODUKCIJE LIPIDOV Z ALGO *CHLORELLA VULGARIS* V RAZLIČNIH MEDIJIH Z VGRADITVIJO OGLJIKOVEGA DIOKSIDA IZ DIMNIH PLINOV V BIOMASO

Prispevki na mednarodnih konferencah:

– Berce P., Golob J., Likozar B.: Rast mikroalge Chlorella vulgaris pod različnimi svetlobnimi režimi / Growth of microalgae Chlorella vulgaris under different exposures to light, Slovenski kemijski dnevi 2010, 23. in 24. september 2010, Maribor. strani 1–6.

RAZISKAVE INDUSTRIJSKIH PROCESOV Z NAMENOM EKOLOŠKE IN ENERGETSKE OPTIMIZACIJE

Prispevki na mednarodnih konferencah:

– Pivar R., Golob J., Likozar B.: Analiza tehnoloških procesov od parnega reforminga do proizvodnje formaldehida / Analysis of technological processes from steam reforming to formaldehyde production, Slovenski kemijski dnevi 2010, 23. in 24. september 2010, Maribor. strani 1–8.

RAZISKAVE NA PODROČJU INŽENIRSTVA OKOLJU PRIJAZNIH PROIZVODOV

Prispevki na mednarodnih konferencah:

– Nograšek B., Golob J., Likozar B.: Načrtovanje integriranega procesa oplaščanja zrn umetnih gnojil in sušenja v fluidiziranem sloju / Design of integrated process of synthetic fertilizer coating process and drying in fluidized bed, Slovenski kemijski dnevi 2010, 23. in 24. september 2010, Maribor. strani 1–11.
– Kavšek M., Golob J., Likozar B.: Mikroenkapsulacija insekticida s polisečnino / Microencapsulation of insecticide with polyurea, Slovenski kemijski dnevi 2010, 23. in 24. september 2010, Maribor. strani 1–11.
– Lapornik D., Golob J., Likozar B.: Ravnotežje in prenos snovi pri sušenju agarnih gelov za pripravo rodenticida / Equilibrium and mass transfer during drying of agar gels for rodenticide preparation, Slovenski kemijski dnevi 2010, 23. In 24. september 2010, Maribor. strani 1–10.
– Prinčič T., Golob J., Strupi-Šuput J., Koglot K., Cotič Z.: Vpliv dodatka superplastifikatorja in elektrofiltrskega pepela na lastnosti cementnih malt, Konferenca Beton 21. stoletja, marec 2010, Lipica.

Raziskava poteka v skladu s programom, podprta je s številnimi publikacijami in prispevki na mednarodnih srečanjih, v okviru programa pa sta v letu 2009 zaključila doktorsko delo dva doktoranda, Nejc Zakrajšek in Jože Šrekl, v tekočem delu pa so vezani na program trije doktorandi in številni diplomanti. V tesni navezavi z industrijskimi obrati prenašamo znanja, ustvarjena v okviru programske skupine, v Unichem, Vrhnika, Nafta Petrochem, Lendava, in IAK, Kresnice.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

TECHNOLOGY OF LIPID PRODUCTION BY *CHLORELLA VULGARIS* ALGAE IN DIFFERENT MEDIA BY INCORPORATION OF CARBON DIOXIDE ORIGINATING FROM FLUE GASES

Environmental protection and depletion of fossil fuel resources are becoming the most important challenges for oil industry, and consequently the whole world. Fossil fuel combustion is the main cause of greenhouse gases, responsible for global warming. To prevent, or at least postpone the inevitably approaching oil crisis and the dramatic climate changes, renewable, low-level carbon and economically achievable energy sources are vitally important. Nowadays, a relatively small part of liquid fuels used for transportation is obtained from oil-rich plants, while photosynthesis of oil-rich algae is still a matter of intensive research all over the world. The purpose of our research was to establish the suitability of microalgae *Chlorella vulgaris* for lipid production. Therefore, optimal process conditions were determined in order to achieve maximum possible oil yield measured as fraction of oil in algae product and overall biomass in algae. Optimization of nutrient supply, study of algae growth, as well as oil production time, and extraction of oil from algae biomass, are only some of the research topics motivating our further work. This research is oriented towards capturing CO_2 originating from flue gases and/or atmosphere in terms of acquiring energy-rich biomass.

RESEARCH OF INDUSTRIAL PROCESSES FOR THEIR ENVIRONMENTAL ACCEPTANCE AND ENERGY-USE IMPROVEMENT

Following the programme goals of atmospheric carbon dioxide reduction and drawing upon the knowledge about minimization of carbon dioxide emissions, various technological problems were examined in order to obtain the results leading towards better technological solutions for the processes in question. Specifically, closing water circuit loops in pulp and paper industry, biodiesel production technology and fire prevention, were studied.

PRODUCT ENGINEERING RESEARCH FOR SUSTAINABLE DEVELOPMENT

This segment of our research programme was characterised by higher added value-oriented research. Studies of this kind demanded examination of the synthesis, analytics, separation techniques, process kinetics and other aspects, with the intention of governance over modelling and optimization of process time considering the parametric sensitivity and transfer of laboratory process to pilot scale.

RESEARCH TOPICS

Technology of lipid production by Chlorella vulgaris algae in different media by incorporation of carbon dioxide originating from flue gases

- CO_2 reduction in flue gases
- production of lipids using *Chlorella vulgaris*

– process condition optimization
– process modelling
– process scale-up and its transfer from laboratory to pilot plant level

Research of industrial processes for their environmental acceptance and energy-use improvement

– study of critical phases of process
– reduction of specific energy consumption per product unit
– reduction of specific CO_2 emissions per product unit
– reduction of production costs per product unit
– increase of product added value

Product engineering research for sustainable development

– product development in laboratory conditions
– optimization of process parameters for the production
– process modelling
– process scale-up from laboratory to pilot plant level
– economic evaluation of technological process viability

SCIENTIFIC ACHIEVEMENTS

RESEARCH OF INDUSTRIAL PROCESSES FOR THEIR ENVIRONMENTAL ACCEPTANCE AND ENERGY-USE IMPROVEMENT

Publications:

– Šrekl J., Golob J.: New approach to calculate the probability of ignition, Journal of loss prevention in the process industries, Vol. 24, No. 3 (2011), p.p. 288–291.
– Šrekl J., Golob J.: Impact of the buildings areas on the fire incidence, Acta chimica slovenica, Vol. 57, No. 1 (2010), p.p. 118–122.

PRODUCT ENGINEERING RESEARCH FOR SUSTAINABLE DEVELOPMENT

Publications:

– Klofutar B., Golob J., Likozar B., Klofutar C., Žagar E., Poljanšek I.: The transesterification of rapeseed and waste sunflower oils : mass-transfer and kinetics in a laboratory batch reactor and in an industrial-scale reactor/separator setup, Bioresource technology, Vol. 101, No. 10 (2010), p.p. 3333–3344.

OTHER RELEVANT ACHIEVEMENTS

– Golob J.: Kaj lahko pričakujemo od centrov odličnosti?, Zbornik-Državni svet Republike Slovenije, Novo mesto, 2010. p. 7.

TECHNOLOGY OF LIPID PRODUCTION BY *CHLORELLA VULGARIS* ALGAE IN DIFFERENT MEDIA BY INCORPORATION OF CARBON DIOXIDE ORIGINATING FROM FLUE GASES

Contributions at international meetings:

– Berce P., Golob J., Likozar B.: Rast mikroalge Chlorella vulgaris pod različnimi svetlobnimi režimi / Growth of microalgae Chlorella vulgaris under different exposures to light, Slovenski kemijski dnevi 2010, 23. and 24. September 2010, Maribor. p.p. 1–6.

RESEARCH OF INDUSTRIAL PROCESSES FOR THEIR ENVIRONMENTAL ACCEPTANCE AND ENERGY-USE IMPROVEMENT

Contributions at international meetings:

– Pivar R., Golob J., Likozar B.: Analiza tehnoloških procesov od parnega reforminga do proizvodnje formaldehida / Analysis of technological processes from steam reforming to formaldehyde production, Slovenski kemijski dnevi 2010, 23. and 24. September 2010, Maribor. p.p. 1–8.

PRODUCT ENGINEERING REASEARCH FOR SUSTAINABLE DEVELOPMENT

Contributions at international meetings:

– Nograšek B., Golob J., Likozar B.: Načrtovanje integriranega procesa oplaščanja zrn umetnih gnojil in sušenja v fluidiziranem sloju / Design of integrated process of synthetic fertilizer coating process and drying in fluidized bed, Slovenski kemijski dnevi 2010, 23. and 24. September 2010, Maribor. p.p. 1–11.
– Kavšek M., Golob J., Likozar B.: Mikroenkapsulacija insekticida s polisečnino / Microencapsulation of insecticide with polyurea, Slovenski kemijski dnevi 2010, 23. and 24. September 2010, Maribor. p.p. 1–11.
– Lapornik D., Golob J., Likozar B.: Ravnotežje in prenos snovi pri sušenju agarnih gelov za pripravo rodenticida / Equilibrium and mass transfer during drying of agar gels for rodenticide preparation, Slovenski kemijski dnevi 2010, 23. and 24. September 2010, Maribor. p.p. 1–10.
– Prinčič T., Golob J., Strupi-Šuput J., Koglot K., Cotič Z.: Vpliv dodatka superplastifikatorja in elektrofiltrskega pepela na lastnosti cementnih malt, Konferenca Beton 21. stoletja, March, 2010, Lipica.

Our research has been carried out according to the programme. It has been documented by several publications and contributions at international meetings. Two PhD candidates completed their theses within the programme framework, i.e. Nejc Zakrajšek and Jože Šrekl, while another three PhD candidates and several BSc candidates are currently working on programme topics. By active cooperation with industrial partners, (Unichem, Vrhnika, Nafta Petrochem, Lendava, and IAK, Kresnice) the resulting knowledge will be transferred into industrial practice.

ENOTE SKUPNE DEJAVNOSTI

Center za NMR spektroskopijo visoke ločljivosti, Enota za športno vzgojo, Knjižnica fakultete, Založba fakultete in Tajništvo (dekanat) fakultete, so enote, ki izvajajo skupno dejavnost fakultete.

CENTER ZA NMR SPEKTROSKOPIJO

je del nacionalnega centra za NMR spektroskopijo, ki vključuje tudi enoti na Kemijskem inštitutu in Inštitutu Jožef Štefan. Kot infrastrukturni center je namenjen znanstveno-raziskovalni, razvojni in izobraževalni dejavnosti. Dejavnosti se izvajajo na podlagi nacionalnega raziskovalnega in razvojnega programa ter nacionalnega programa visokega šolstva (diplomske, magistrske naloge in doktorske disertacije).

ENOTA ZA ŠPORTNO VZGOJO

skrbi za izvajanje športne vzgoje študentov fakultete.

KNJIŽNICA FAKULTETE

skrbi za izposojo, nabavo in katalogizacijo strokovne literature ter za vnos biografskih in bibliografskih podatkov visokošolskih učiteljev, znanstvenih delavcev in sodelavcev fakultete v COBISS.

ZALOŽBA FAKULTETE

skrbi za izdajo učbenikov in drugega strokovnega gradiva potrebnega za izvajanje izobraževalne ter znanstveno-raziskovalne in razvojne dejavnosti.

TAJNIŠTVO (DEKANAT) FAKULTETE

skrbi za razreševanje organizacijskih in pravnih zadev, za vodenje strokovno-administrativnih opravil s študijskega, znanstveno-raziskovalnega in razvojnega,

personalnega, gospodarsko-finančnega in računovodskega področja, za knjižnico, izdajanje učbenikov in učnih pripomočkov, za vodenje habilitacijskih postopkov, področja varnosti in zdravja pri delu, podporo mednarodnemu sodelovanju, vzdrževanje nepremičnin, vzdrževanje spletnih strani fakultete, vzdrževanje stavb in opreme, delovanje računalniške opreme fakultete in za administrativno-tehnična dela pri izvajanju nacionalnega programa visokega šolstva in nacionalnega raziskovalnega in razvojnega programa. Tajništvo sestavljajo naslednje podenote:

– splošno in strokovno področje,
– računovodsko finančna služba,
– študentski referat,
– kadrovska služba in
– tehnično vzdrževalna skupina.

KATEDRE V LETU 2010
CHAIRS IN 2010


FAKULTETA ZA KEMIJO
5

KATEDRA ZA ANALIZNO KEMIJO
CHAIR OF ANALYTICAL CHEMISTRY

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Marjan Veber

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Boris Pihlar
prof. dr. Marjan Veber
izr. prof. dr. Lucija Zupančič-Kralj
izr. prof. dr. Nataša Gros

Asistenti / Assistants
dr. Robert Susič
dr. Tatjana Zupančič
doc. dr. Matevž Pompe
doc. dr. Helena Prosen
doc. dr. Drago Kočar
dr. Irena Kralj Cigić
dr. Polonca Kralj
mag. Ivanka Keber

Raziskovalci / Researchers
izr. prof. dr. Matija Strlič (v dopolnilnem razmerju / *part-time*)
dr. Martin Šala

Tehniki / Technicians
Zdenka Držaj
Jolanda Furlan
Mojca Žitko

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Tanja Trafela	M. Strlič	2006–2010	doktorski študij/ *PhD*
Andrej Ščavničar	M. Pompe	2007–2012	doktorski študij / *PhD*
Alenka Možir	M. Strlič	2008–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemija / *Chemistry* – UN:
Analizna kemija I, II / *Analytical Chemistry I, II*
Praktikum iz analizne kemije / *Practicum in Analytical Chemistry*
Kemija okolja (izbirni predmet) / *Environmental Chemistry (elective course)*

Biokemija / *Biochemistry* – UN:
Instrumentalne metode analize / *Instrumental Methods of Analysis*

Kemijsko inženirstvo / *Chemical Engineering* – UN:
Intrumentalne metode analize / *Instrumental Methods of Analysis*
Praktikum iz instrumentalnih metod analize / *Practicum in Instrumental Analysis*

Tehniška varnost / *Technical Safety* – UN:
Meritve v delovnem okolju (izbirni predmet) / *Measurements in Work Environment (elective course)*

Kemijska tehnologija / *Chemical Technology* – VS:
Praktikum iz kemije / *General Chemistry – Practical Course*
Analizna kemija I, II / *Analytical Chemistry I, II*
Kemija okolja (izbirni predmet) / *Environmental Chemistry (elective course)*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Analitika in spektroskopija / *Chemical Analysis and Spectroscopy* – VS
Avtomatizirana analiza / *Automated Analysis* – UN
Instrumentalna analiza / *Instrumental Analysis* – UN
Instrumentalne metode analize / *Instrumental Methods in Chemical Analyis* – UN
Izbrana poglavja iz analizne kemije / *Selected Topics in Analytical Chemistry* – UN
Kemija okolja / *Environmental Chemistry* – UN
Kemijska analiza živil / *Food Analysis* – UN
Kemometrija v analizni kemiji / *Chemometrics in Analytical Chemistry* – UN

Bolonjski programi 2. stopnje / *Bologna 2nd Cycle Master Study Programmes*

Tehniška varnost / *Technical Safety:*

Instrumentalna analiza in monitoring (izbirni predmet) */Instrumental Analysis and Monitoring (elective course)*

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Nova področja v analizni kemiji / *New Fields in Analytical Chemistry*

Pristopi v sodobni analizni kemiji / *Approaches in Modern Analytical Chemistry*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Analizna kemija FFA – Farmacija UN in Laboratorijska biomedicina UN / *Analytical Chemistry / Uniform Master Study Programme in Pharmacy and Undergraduate Study Programme in Laboratory Biomedicine*

Analizna kemija / *Analytical Chemistry* PEF – UN

Kemija okolja / *Environmental Chemistry* PEF – UN

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Analizna kemija v kontroli okolja / *Analytical Chemistry in Environmental Control* – UL Interdisciplinarni doktorski študijski program Varstvo okolja / *UL Interdisciplinary Doctoral Study Programme in Environmental Protection*

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

Temeljna raziskovalna dejavnost je razvoj novih analiznih metod, postopkov in instrumentacije ter študij reakcijskih sistemov in ravnotežij, pomembnih v analizni kemiji. Med pomembnejša raziskovalna področja spadajo kromatografija, spektroskopija, elektroanalizne tehnike, pretočna analiza, kemometrija ter avtomatizirana in robotizirana analiza.

Področja, ki jim posvečamo več pozornosti, so zlasti študij interakcij med kovinami in antibiotiki/kemoterapevtiki, pesticidi in huminskimi substancami; raziskave in opredeljevanje kemijskih zvrsti; raziskave vloge prehodnih kovin v oksidativnih medijih; karakterizacija in stabilizacija organskih materialov, zlasti polimernih; študij elektrodnih procesov in razvoj voltametričnih analiznih tehnik ter senzorjev; študij separacijskih in predkoncentracijskih postopkov (dializa, ekstrakcija na trdni fazi); analitika živil, (vina, mesa in sira); analitika sledov kovin; razvoj postopkov atomske spektroskopije (AAS, ICP-MS); atmosferska kemija ter konzervacijska kemija; uporabe kemometričnih pristopov v analizni kemiji.

Research activities of the Department of Analytical Chemistry are focused on the development of new analytical procedures and instrumentation as well as studies of important equilibria in analytical chemistry. Main research topics include: chromatography, spectroscopy, electroanalytical techniques, flow injection analysis, chemometry, automated analysis and robotics in analytical chemistry.

Our research focuses on studying interactions between metals and antibiotics, pesticides, humic substances, speciation studies and the role of transition elements in oxidative media, char-

acterization and stabilization of organic matter with special focus on polymers, studies of processes on electrodes and development of new voltammetric techniques and sensors, studies of separation and preconcentration procedures (dialysis, solid phase extraction), food analysis (wine products, meat products and cheese), development of methods and procedures in atomic spectroscopy (AAS ICP-MS), atmospheric chemistry and chemical studies of preservation of cultural heritage; the application of chemometric approaches in analytical chemistry.

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

M. Veber, pohvala Študentskega sveta za pedagoško delo na smeri Biokemija / *Students Award for the Quality of Teaching in Biochemistry Study Programme*

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

- M. Veber, M. Strlič, B. Pihlar, *Acta Chimica Slovenica*
- M. Veber, *Chemia Analityczna*
- M. Strlič, J. Kolar, *e-Preservation Science*
- M. Strlič, *Papir*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Sklopljeni instrument plinski kromatograf-masni spektrometer Hewlett-Packard mod. 5990 A / GC-MS / *Gas Chromatograph with Mass-Spectrometric Detection Hewlett-Packard Mod. 5989 A/ GC-MS*
- Plinski kromatograf s kvadrupolnim masnim spektrometrom GC: Agilent Technologies 7890A, MS: Agilent Technologies 5975C / *Gas Chromatograph with Mass-Spectrometric Detection Agilent Technologies 7890A, MS Agilent Technologies 5975C*
- Sklopljeni instrument plinski kromatograf – masni spektrometer Varian mod. Saturn 2000 / GC-MS / *Gas Chromatograph with Mass-Spectrometric Detection Varian Mod. Saturn 2000 / GC – MS*
- Plinski kromatograf z ECD in FID detektorjema HP 6890 / *Gas Chromatograph with ECD and FID Detectors HP 6890*
- Robotski sistem Zymark Prelude / *Benchtop Robotic System Zymark Prelude*
- Kemiluminometer / *Chemilluminometer*
- 3 HPLC kromatografski sistemi HP 1100 / 3 *HPLC- Systems (Hewlett Packard 1100 Series)*
- Potenciostat/Galvanostat M283, M273, EG&G PARC
- FAAS-ETAAS Perkin Elmer

– Atomski absorpcijski spektrometer PerkinElmer AAnalyst 600 */AAS Spectrometer Perkin Elmer AAnalyst 600*
– Ionski kromatograf-Dionex DX 500 / *Ion Chromatograph*
– Avtotitator Metrohm, Tinet / *Autotitrator*
– Kapilarna elektroforeza-Applied Biosystems, 270A-HT / *Capillary Electrophoresis*
– Klimatska komora / *Climate Chamber Vötsch 0030*
– FTIR Perkin Elmer 1000
– IR spektrometer ADS Labspec 5000 / *IR Spectrometer ADS Labspec 5000*
– UV-VIS Varian Cary 50 spektrofotometer / *Spectrophotometer*
– Spektrofluorimeter Varian Cary Elipse */ Spectrofluorimeter Varian Cary Elipse*

Skupaj z NUK / *Shared with the National and University Library*:
– FT-NIR-MidIR-IR Perkin Elmer GX/ z DRIFT NIR celico / *with a DRIFT NIR Cell*
– Pretočni analizni sistem za viskozimetrijo / *Flow Analysis System for Viscometry*

Skupaj s KI / *Shared with the National Institute of Chemistry*:
– ICP-MS HP (Agilent) 4500
– ICP-MS-LA Agilent 7500 CE - UP-213

Skupaj z UNG in Kmetijskim inštitutom Slovenije / *Shared with the University of Nova Gorica and the Agricultural Institute of Slovenia*
– Sklopljeni tekočinski kromatograf/ masni spektrometer / *HPLC-MS /MS (Perkin Elmer Series 200, Applied Biosystems 3200 Q Trap)*

SODELOVANJE V CENTRIH ODLIČNOSTI / CENTERS OF EXCELLENCE

– Center odličnosti: Nanoznanosti in nanotehnologija / *Center of Excellence: Nanosciences and Nanotechnology*
– Center odličnosti: Polimerni materiali (PoliMat) / *Center of Excellence: Polymeric Materials (PoliMat)*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P1–0153 Raziskave in razvoj analiznih metod in postopkov / *Research and Development of Analytical Methods and Procedures*
Vodja programa / *Principal Researcher*: B. Pihlar

MEDNARODNO SODELOVANJE NA PODROČJU IZOBRAŽEVANJA / INTERNATIONAL COOPERATION IN EDUCATION

CEEPUS CII PL-0004-02-0607
Education in Separation and Identification of Organic Xenobiotics in Environmental Samples and Food Products
Koordinator / *Coordinator*: M. Veber

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

LLP-LDV-TOI-2008-SUI-15	*Hands-on Approach to Analytical Chemistry for Vocational Schools (II)* Nosilka / *Principal Researcher*: N. Gros
COST D42	*Chemical Interactions between Cultural Artefacts and the Indoor Environment – EnviArt* Nosilec / *Principal Researcher*: M. Strlič
FOOD-CT 2006-06264 EU 6.OP	*Traditional Europe Food (TRUEFOOD)* Nosilec / *Principal Researcher*: M. Pompe

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Hrvaška *Slovenia – Croatia*	Nastanek, transport in razgradnja fotooksidantov na področju Mediterana / *Formation, Transport and Degradation of Photooxidants in the Mediterranean* Nosilec / *Principal Researcher*: M. Pompe
Slovenija – Kitajska *Slovenia – China*	Onesnaževala povezana s prometom: ocena virov emisij in tvorbenih mehanizmov aerosolov / *Transportation-Related Pollutants: Estimation of Emission Sources and Formation Pathways of Aerosols* Nosilec / *Principal Researcher*: M. Pompe
Slovenija – ZDA *Slovenia – USA*	Kvantitativna ocena tveganja pri tradicionalnih izdelkih živil / *Quantitative Risk Assessment of Traditional Food Products* Nosilec / *Principal Researcher*: M. Veber
Slovenija –Turčija *Slovenia – Turkey*	Sistem nadzora in sledljivosti biogenih aminov in nitrozamina v tradicionalnih ribjih produktih / *Systems of Control and Traceability of Biogenetic Amines and Nitrosamines in Traditional Fish Products* Nosilec / *Principal Researcher*: M. Pompe

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

AL1. BUBNIČ, Zoran, URLEB, Uroš, KREFT, Katjuša, VEBER, Marjan. Determination of nickel in active pharmaceutical ingredients by electrothermal atomic absorption spectrometry. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 37–44. [COBISS.SI-ID 33810437]

AL2. ARH, Gregor, KLASINC, Leo, VEBER, Marjan, POMPE, Matevž. Modeling of the mass spectrometric response factors in non-target analysis. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 3, str. 581–585. [COBISS.SI-ID 34555141]

AL3. GROS, Nataša, CAMÕES, Maria Filomena, SILVA, Ricardo J. N. Bettencourt da. Detailed uncertainty budget for major and minor ions in stock combined calibration standards : influence of impurities in chemicals. *Anal. chim. acta*. [Print ed.], 2010, vol. 659, no. 1/2, str. 85–92. [COBISS.SI-ID 33467909]

AL4. GROS, Nataša, CAMÕES, Maria Filomena, SILVA, Ricardo J. N. Bettencourt da. Uncertainty budget for simultaneous determination of minor and major ions in seawater with ion chromatography confronted with uncertainties in concentrations of calibration standards. *Anal. lett.*, 2010, vol. 43, no. 7/8, str. 1317–1329. [COBISS.SI-ID 34056197]

AL5. FENECH, Ann, STRLIČ, Matija, KRALJ CIGIĆ, Irena, LEVART, Alenka, GIBSON, Lorraine, BRUIN, G. de, NTANOS, Kostas, KOLAR, Jana, CASSAR, May. Volatile aldehydes in libraries and archives. *Atmos. environ. (1994)*. [Print ed.], 2010, vol. 44, no. 17, str. 2067–2073. [COBISS.SI-ID 33984261]

AL6. JANEŠ, Damjan, PROSEN, Helena, KREFT, Ivan, KREFT, Samo. Aroma compounds in buckwheat (Fagopyrum esculentum Moench) groats, flour, bran, and husk. *Cereal chem.*, 2010, vol. 87, no. 2, str. 141–143. [COBISS.SI-ID 2763121]

AL7. ŠALA, Martin, KITAHARA, Yuki, TAKAHASHI, Seiji, FUJII, Toshihiro. Effect of atmosphere and catalyst on reducing bisphenol A (BPA) emission during thermal degradation of polycarbonate. *Chemosphere (Oxford)*. [Print ed.], 2010, vol. 78, no. 1, str. 42–45. [COBISS.SI-ID 33377285]

AL8. STRLIČ, Matija, KRALJ CIGIĆ, Irena, MOŽIR, Alenka, THICKETT, David, BRUIN, G. de, KOLAR, Jana, CASSAR, May. Test for compatibility with organic heritage materials : a proposed procedure. *E-preservation science*, 2010, vol. 7, str. 78–86. [COBISS.SI-ID 34215173]

AL9. PIECHA, Malgorzata, SARAKHA, Mohamed, TREBŠE, Polonca, KOČAR, Drago. Stability studies of cholesterol lowering statin drugs in aqueous samples using HPLC and LC-MS. *Environ. chem. lett. (Tiskan)*, 2010, issue 2, vol. 8, str. 185–191. [COBISS.SI-ID 1070587]

AL10. BEESTON, Michael Philip, POHAR, Andrej, ELTEREN, Johannes Teun van, PLAZL, Igor, ŠLEJKOVEC, Zdenka, VEBER, Marjan, GLASS, Hylke J. Assessment of physical leaching processes of some elements in soil upon ingestion by continuous leaching and modeling. *Environ. sci. technol.*. [Print ed.], 2010, vol. 44, issue 16, str. 6242–6248.[COBISS.SI-ID 4448538]

AL11. MODEC, Barbara, ŠALA, Martin, CLÉRAC, Rodolphe. Pyrazine-assisted dimerization of molybdenum(V) : synthesis and structural characterization of novel dinuclear and tetranuclear complexes. *European Journal of Inorganic Chemistry*, 2010, no. 4, str. 542–553. [COBISS.SI-ID 33587973]

AL12. PROSEN, Helena, KOKALJ, Meta, JANEŠ, Damjan, KREFT, Samo. Comparison of isolation methods for the determination of buckwheat volatile compounds. *Food chem.*. [Print ed.], 2010, vol. 121, no. 1, str. 298–306. [COBISS.SI-ID 33728005]

AL13. SABLIER, Michel, ŠALA, Martin, KITAHARA, Yuki, TAKAHASHI, Seiji, FUJII, Toshihiro. Influence of copper chloride for the formation of aromatic compounds during polyethylene pyrolysis. *J. anal. appl. pyrolysis*. [Print ed.], 2010, vol. 89, no. 2, str. 178–182. [COBISS.SI-ID 34405125]

AL14. PEČKO, Darja, ŽUŽEK ROŽMAN, Kristina, MCGUINESS, Paul J., PIHLAR, Boris, KOBE, Spomenka. Temperature-driven microstructural, compositional, and magnetic changes in electrodeposited Fe-Pd thin films. *J. appl. phys.*, 2010, vol. 107, no. 9, str. 09A712-1-97A712-3. [COBISS.SI-ID 23550759]

AL15. TOPORIŠIČ, Rebeka, MLAKAR, Anita, HVALA, Jernej, PRISLAN, Iztok, ZUPANČIČ-KRALJ, Lucija. Identification of new impurities of enalapril maleate on oxidation in the presence of magnesium monoperoxyphthalate. *J. pharm. biomed. anal.*. [Print ed.], 2010, vol. 52, no. 2, str. 294–299. [COBISS.SI-ID 34108677]

AL16. ŽAKELJ, Simon, BERGINC, Katja, URŠIČ, Darko, VEBER, Marjan, KRISTL, Albin. Metal cation-fluoroquinolone complexes do not permeate through the intestinal absorption barrier. *J. pharm. biomed. anal.*. [Print ed.], 2010, vol. 53, iss. 3, str. 655–659. [COBISS.SI-ID 2854257]

AL17. STRMČNIK, Dušan, HODNIK, Nejc, HOČEVAR, Samo B., VLIET, D. van der, ZORKO, Mateja, STAMENKOVIC, Vojislav, PIHLAR, Boris, MARKOVIC, Nenad M. Novel method for fast characterization of high-surface-area electrocatalytic materials using a carbon fiber microelectrode. *The journal of physical chemistry. C, Nanomaterials and interfaces*, 2010, vol. 114, no. 17, str. 2640–2644. [COBISS.SI-ID 4384794]

AL18. MURKO, Simona, MILAČIČ, Radmila, VEBER, Marjan, ŠČANČAR, Janez. Determination of Cd, Pb and As in sediments of the Sava River by electrothermal atomic absorption spectrometry. *J. Serb. Chem. Soc.*, 2010, vol. 75, no. 1, str. 113–128. [COBISS.SI-ID 23362599]

AL19. HUREMOVIĆ, Jasna, HORVAT, Milena, VEBER, Marjan, MEMIĆ, Mustafa. Kontrola polutanata u zraku uporabom epifitskog lišaja Hypogymnia physodes u Sarajevu, Bosna i Hercegovina. *Kem. ind.*. [Print ed.], 2010, vol. 59, no. 3, str. 107–110. [COBISS.SI-ID 23439399]

AL20. BUDIJA, Franc, ZUPANČIČ-KRALJ, Lucija, PETRIČ, Marko. Optimizacija utekočinjanja biomase z glicerolom in karakterizacija nastalih hlapnih produktov = Optimisation of biomass liquefaction with glycerol and characterisation of theformed volatile products. *Les (Ljubl.)*, 2010, let. 62, št. 5, str. 209–215. [COBISS.SI-ID 1809801]

AL21. ULČNIK, Ajda, ZUPANČIČ-KRALJ, Lucija, TAVZES, Črtomir, POHLEVEN, Franc. Mikoremediacija lindana v tekočih kulturah gliv Pleurotus ostreatus in Hypoxlon fragiforme = Mycoremediation of lindane in liquid cultures of Pleurotus ostreatus and Hypoxylon fragiforme. *Les (Ljubl.)*, 2010, let. 62, št. 5, str. 216–221. [COBISS.SI-ID 1810057]

AL22. STRLIČ, Matija, MENART, Eva, KRALJ CIGIĆ, Irena, KOLAR, Jana, BRUIN, G. de, CASSAR, May. Emission of reactive oxygen species during degradation of iron gall ink. *Polym. degrad. stab.*. [Print ed.], 2010, vol. 95, no. 1, str. 66–71. [COBISS.SI-ID 33496837]

AL23. THOMAS, Jacob, TOWNSEND, J. H., HACKNEY, Stephen, STRLIČ, Matija. A chemiluminescence study of madder lakes on paper. *Polym. degrad. stab.*. [Print ed.], 2010, vol. 95, no. 12, str. 2343–2349. [COBISS.SI-ID 34622469]

AL24. FENECH, Ann, STRLIČ, Matija, DEGANO, Ilaria, CASSAR, May. Stability of chromogenic colour prints in polluted indoor environments. *Polym. degrad. stab.*. [Print ed.], 2010, vol. 95, no. 12, str. 2481–2485. [COBISS.SI-ID 34621957]

AL25. STRLIČ, Matija, CSEFALVAYOVA, Linda, KOLAR, Jana, MENART, Eva, KOSEK, Joanna M., BARRY, Caroline, HIGGITT, Catherine, CASSAR, May. Non-destructive characterisation of iron gall ink drawings : not such a galling problem. *Talanta (Oxford)*. [Print ed.], 2010, vol. 81, no. 1/2, str. 412–417. [COBISS.SI-ID 33743365]

AL26. CSEFALVAYOVA, Linda, PELIKAN, M., KRALJ CIGIĆ, Irena, KOLAR, Jana, STRLIČ, Matija. Use of genetic algorithms with multivariate regression for determination of gelatine in historic papers based on FT-IR and NIR spectral data. *Talanta (Oxford)*. [Print ed.], 2010, vol. 82, no. 5, str. 1784–1790. [COBISS.SI-ID 34458629]

AL27. LESAR, Boštjan, HUMAR, Miha, KRALJ, Polonca. Influence of montan wax emulsions on leaching dynamics of boric acid from impregnated wood. *Wood research*, 2010, let. 55, št. 1, str. 93–100. [COBISS.SI-ID 1792649]

AL28. IVEKOVIĆ, Damir, GAJOVIĆ, Andreja, ČEH, Miran, PIHLAR, Boris. Prussian blue-modified titanate nanotubes : A novel nanostructured catalyst for electrochemical reduction of hydrogen peroxide. *Electroanalysis*, 2010, vol. 22, no. 19, str. 2202–2210. [COBISS.SI-ID 24239655]

AL29. LESAR, Boštjan, KRALJ, Polonca, HUMAR, Miha. Influence of polyethylene and oxidized polyethylene wax emulsions on leaching dynamics of boric acid from impregnated spruce wood. *Drv. ind.*, 2010, vol. 61, br. 4, str. 213–221. [COBISS.SI-ID 1871241]

AL30. KLASINC, Leo, CVITAŠ, Tomislav, DE MARCO, Alessandra, KEZELE, Nenad, PAOLETTI, Elena, POMPE, Matevž. Rating of Mediterranean photochemical air pollution monitoring sites. *Fresenius environ. bull.*. [Print ed.], 2010, vol. 19, no. 9B, str. 1982–1988. [COBISS.SI-ID 34920197]

KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

AL31. NEMEČEK, Nataša, CSEFALVAYOVA, Linda, STRLIČ, Matija. Identifikacija roževine, slonovine in kosti z metodo bližnje infrardeče spektroskopije (NIR). *Argo*, 2010, [Letn.] 53, [št.] 1, str. 114–117. [COBISS.SI-ID 7680352]

AL32. PETERLIN, Simona, TRAFELA, Tanja, STRLIČ, Matija, DRNOVŠEK, Tjaša, KOLAR, Jana. Uporaba FT-(N)IR spekttroskopije pri spremljanju procesa mletja papirniških vlaken = Use of FT-(N)IR spectroscopy to monitor the beating process of papermaking fibres. *Papir (Ljubl.)*, maj 2010, letn. 38, št. 3, str. 30–32, ilustr. [COBISS.SI-ID 350144]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

AL33. GROS, Nataša. Small-scale analytical devices for the at-line monitoring of biotechnological processes. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–5]. [COBISS.SI-ID 34497285]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

AL34. KRALJ CIGIĆ, Irena, STRLIČ, Matija, BRUIN, G. de, KOLAR, Jana, STEEMERS, Ted. VOCs in paper-based cultural heritage collections - source of information or risk?. V: *Impact of the indoor environment on the preservation of our movable heritage : ENVIART*. [S. l.: s. n.], 2010, str. 63–65. [COBISS.SI-ID 34599429]

AL35. RABIN, Ira, KRALJ CIGIĆ, Irena, STRLIČ, Matija. Dead Sea Scrolls studies in the frame of COST D42. V: *Impact of the indoor environment on the preservation of our movable heritage : ENVIART*. [S. l.: s. n.], 2010, str. 66–68. [COBISS.SI-ID 34599685]

AL36. STRLIČ, Matija, LOJEWSKI, Tomasz. Overview of WG2 activities in COST D42 : analysis of heritage materials and environments. V: *Impact of the indoor environment on the preservation of our movable heritage : ENVIART*. [S. l.: s. n.], 2010, str. 93–97. [COBISS.SI-ID 34599941]

AL37. MOŽIR, Alenka, STRLIČ, Matija, TRAFELA, Tanja, KRALJ CIGIĆ, Irena, KOLAR, Jana, DESELNICU, Viorica. Characterisation of historic parchment using near infrared spectroscopy. V: *Impact of the indoor environment on the preservation of our movable heritage : ENVIART*. [S. l.: s. n.], 2010, str. 119–121. [COBISS.SI-ID 34602501]

AL38. STRLIČ, Matija, BRIMBLECOMBE, Peter, BELL, Nancy, TAYLOR, Joel, XUE, Jinghao, THICKETT, David, FRANCE, Fenella. Collections demography – on dynamic evolution of populations of objects. V: *Impact of the indoor environment on the preservation of our movable heritage : ENVIART*. [S. l.: s. n.], 2010, str. 125–126. [COBISS.SI-ID 34602757]

AL39. KRALJ CIGIĆ, Irena, KOLAR, Jana. Research activities in Slovenia related to COST action D42 2006-2010. V: *Impact of the indoor environment on the preservation of our movable heritage : ENVIART*. [S. l.: s. n.], 2010, str. 140–142. [COBISS.SI-ID 34603013]

AL40. HUMAR, Miha, LESAR, Boštjan, UGOVŠEK, Aleš, KARIŽ, Mirko, KRALJ, Polonca, ŠERNEK, Milan. Influence addition of boron compounds to adhesives on the bonding quality and fungicidal properties of glued wood. V: *IRG 41 Annual Meeting, Biarritz, France, 9 May 2010*. [Biarritz]: IRG, 2010, 11 str. [10–40497.pdf]. [COBISS.SI-ID 1811849]

AL41. BRUIN, G. de, STRLIČ, Matija, KRALJ CIGIĆ, Irena. Smell of books and paper: indicator of physical condition? : [lecture]. V: COST D42 WG2 Meeting, National Library of Spain, Madrid, Spain, 11–12 March, 2010. *»Preservation and challenges in libraries, museums and archives: environmental controls and analytical diagnostics«*. [S. l.: s. n.], 2010, str. [1–2]. [COBISS.SI-ID 33866245]

AL42. STRLIČ, Matija. Paper heritage: overview of recent European research projects : [lecture]. V: COST D42 WG2 Meeting, National Library of Spain, Madrid, Spain, 11–12 March, 2010. *»Preservation and challenges in libraries, museums and archives: environmental controls and analytical diagnostics«*. [S. l.: s. n.], 2010, str. [1–3]. [COBISS.SI-ID 33865989]

AL43. GROS, Nataša. Bridging the gap in lack of professional instrumentation – small scale, low-cost analytical instruments for greater equity in learning analytical chemistry. V: DOLINŠEK, Slavko (ur.). XIV. IOSTE Symposium, International Organization for Science and Technology Education, June 13.–18. 2010, Bled, Slovenia. *Socio-cultural and human values in science and technology education : proceedings*. Ljubljana: Institute for Innovation and Development of University, 2010, str. 1–2. [COBISS.SI-ID 34184709]

AL44. GROS, Nataša, VRTAČNIK, Margareta. European project transfer of inovation »Hands-on Approach to Analytical Chemistry for Vocational Schools« = Evropski projekt prenosa inovacij »Izkustveni pristop k analizni kemiji za strokovne šole«. V: DOLINŠEK, Slavko (ur.). XIV. IOSTE Symposium, International Organization for Science and Technology Education, June 13.–18. 2010, Bled, Slovenia. *Socio-cultural and human values in science and technology education : proceedings*. Ljubljana: Institute for Innovation and Development of University, 2010, str. [1–2]. [COBISS.SI-ID 34184453]

UNIVERZITETNI ALI VISOKOŠOLSKI UČBENIK Z RECENZIJO / REVIEWED UNIVERSITY AND ACADEMIC TEXTBOOK

AL45. PIHLAR, Boris. *Osnove analizne kemije : zapiski predavanj*. (Ponatis). Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2008–. Zv. <1>, ilustr. ISBN 978-961-6286-42-8. ISBN 978-961-6286-43-5. [COBISS.SI-ID 235267840]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

AL46. PROSEN, Helena, SUSIČ, Robert. *Laboratorijski seminar iz Analizne kemije I : verzija 1.0 : za 1. letnik univerzitetnega študija kemija : Elektronski vir*. Ljubljana: [H. Prosen, R. Susič], 2010. 53 str., ilustr. [COBISS.SI-ID 34434053]

AL47. PROSEN, Helena, KRALJ CIGIĆ, Irena, STRLIČ, Matija. *Praktikum iz analizne kemije : verzija 1.0 : za 2. letnik univerzitetnega študija kemija : Elektronski vir*. Ljubljana: [H. Prosen], 2010. 97 str., ilustr. [COBISS.SI-ID 34440453]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

AL48. STRLIČ, Matija, KRALJ CIGIĆ, Irena, PIHLAR, Boris, KOLAR, Jana, BRUIN, G. de, STEEMERS, Ted. *Final activity report : confidential : PaperVOC : L1-9710-0103-06 : volatile organic compounds in paper-based cultural heritage collections – source of information or health risk?*. Ljubljana: Univ. v Ljubljani, 2010. 1 zv. (loč. pag.), ilustr. [COBISS.SI-ID 33831685]

PATENT / PATENT

AL49. ANDERS, Manfred, LICHTBLAU, Dirk Andreas, KOLAR, Jana, MALEŠIČ, Jasna, STRLIČ, Matija, ŠALA, Martin, KOČEVAR, Marijan. *Antioxidant for an organic material and method for treating the same : patent : EP 1664431 (B1), 2010-08-04*. [S. l.]: European Patent Office, 2010. 21 str., ilustr. [COBISS.SI-ID 26939909]

UREDNIK / EDITORSHIP

AL50. *Acta chimica slovenica*. Strlič, Matija (urednik 2003–, gostujoči urednik 2007), Pihlar, Boris (član uredniškega odbora 1998–), Veber, Marjan (član uredniškega odbora 1998–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [COBISS.SI-ID 14086149]

AL51. *E-preservation science*. Strlič, Matija (urednik 2004–). Ivančna Gorica: Morana RTD, 2004–. ISSN 1581-9280. [COBISS.SI-ID 214150912]


FAKULTETA ZA KEMIJO

KATEDRA ZA ANORGANSKO KEMIJO
CHAIR OF INORGANIC CHEMISTRY

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Iztok Turel

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Nataša Bukovec
prof. dr. Peter Bukovec
izr. prof. dr. Boris Čeh
prof. dr. Alojz Demšar
prof. dr. Ivan Leban
prof. dr. Anton Meden
doc. dr. Barbara Modec
doc. dr. Saša Petriček
prof. dr. Iztok Turel

Asistenti / Assistants
doc. dr. Romana Cerc Korošec
Nataša Čelan Korošin, univ. dipl. kem.
doc. dr. Amalija Golobič
dr. Sabina Grabner
dr. Nives Kitanovski
dr. Irena Kozjek Škofic
doc. dr. Bojan Kozlevčar
doc. dr. Nina Lah
doc. dr. Andrej Pevec
dr. Elizabeta Tratar Pirc
doc. dr. Marija Zupančič
doc. dr. Franc Perdih
Katarina Stare, univ. dipl. kem.

Tehniki / Technicians

Damjan Erčulj
Karmen Klančar
Aleš Knez
Urška Levec
Petra Vuković
Igor Ponikvar

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Simona Medvešček	A. Meden	2003–2010	doktorski študij / *PhD*
Jerneja Šauta Ogorevc	P. Bukovec	2006–2011	doktorski študij / *PhD*
Marta Kasunič	A. Golobič	2007–2012	doktorski študij / *PhD*
Rosana Hudej	I. Turel	2008–2012	doktorski študij / *PhD*
Jakob Kljun	I. Leban	2008–2012	doktorski študij / *PhD*
Ksenija Cer Kerčmar	P. Bukovec	2009–2013	doktorski študij / *PhD*
Maja Vidmar	A. Golobič	2009–2013	doktorski študij/ *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemija / *Chemistry* – UN:

Splošna kemija / *General Chemistry*

Praktikum iz splošne in anorganske kemije / *Practicals in General and Inorganic chemistry*

Anorganska kemija / *Inorganic Chemistry*

Zgradba in lastnosti trdnin / *Structure and Properties of Solids*

Spektroskopija / *Spectroscopy*

Anorganska sinteza (izbirni predmet) / *Inorganic Synthesis (elective course)*

Kemija za trajnostni razvoj (izbirni predmet) / *Chemistry for Sustainable Development (elective course)*

Anorganska kemija II (izbirni predmet) / *Inorganic Chemistry II (elective course)*

Biokemija / *Biochemistry* – UN:

Splošna kemija / *General Chemistry*

Kemijski praktikum / *Practicals in Chemistry*

Anorganska kemija / *Inorganic Chemistry*

Kemijsko inženirstvo / *Chemical Engineering* – UN:

Splošna kemija / *General Chemistry*
Anorganska kemija / *Inorganic Chemistry*

Praktikum iz splošne in anorganske kemije / *Practicals in General and Inorganic Chemistry*

Tehniška varnost / *Technical Safety* – UN:
Kemija / *Chemistry*

Gorenje in dinamika požarov / *Fire and Fire Dynamics*

Kemijska tehnologija / *Chemical Technology* – VS:

Splošna kemija I / *General Chemistry I*

Splošna kemija II / *General Chemistry II*

Anorganska kemija I / *Inorganic Chemistry I*

Anorganska kemija II / *Inorganic Chemistry II*

Praktikum iz kemije / *General Laboratory Practice*

Sintezne metode v anorganski kemiji (izbirni predmet) / *Methods of Syntheses in Inorganic Chemistry (elective course)*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Anorganska kemija II / *Inorganic Chemistry II* – UN

Bioanorganska kemija / *Bioinorganic Chemistry* – UN

Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UN

Izbrana poglavja iz anorganske kemije / *Selected Topics in Inorganic Chemistry* – UN

Kristalna kemija / *Crystal Chemistry* – UN

Metodika anorganskih eksperimentov / *Methodology of Inorganic Experiments* – UN

Kemija kompleksov / *Coordination Chemistry* – UN

Teorija gorenja, gašenja in dinamika požarov / *Theory of Combustion, Extinction and Fire Dynamics* – VS

Anorganska kemija / *Inorganic Chemistry* – VS

Splošna kemija / *General Chemistry* – VS

Bolonjski programi 2. stopnje / *Bologna 2nd Cycle Master Study Programmes*

Tehniška varnost / *Technical Safety:*

Požarna varnost (izbirni predmet skupine A) / *Fire Safety (elective course)*

Požarnovarnostna analiza objektov (izbirni predmet skupine B) / *Fire Safety Analysis of Constructions (elective course)*

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Izbrana poglavja iz anorganske kemije / *Selected Topics in Inorganic Chemistry*

Sodobne metode sinteze v anorganski kemiji / *Synthesis and Reactivity of Inorganic Compounds*

Sodobne difrakcijske tehnike / *Contemporary Diffraction Techniques*

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Koordinacijska kemija / *Coordination Chemistry*
Rentgenska strukturna analiza / *X-ray Structure Analysis*
Aplikativna kristalografija / *Applied Crystallography*
Kemija trdnega stanja / *Solid State Chemistry*
Organokovinska kemija / *Metal-Organic Chemistry*
Termična analiza / *Thermal Analysis*
Bioanorganska kemija / *Bioinorganic Chemistry*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemija / *Chemistry* FS – UN
Kemija I, II / *Chemistry I, II* NTF – UN
Anorganska kemija I, II / *Inorganic Chemistry I, II* NTF – UN
Kemija I, II / *Chemistry I, II* FMF – UN
Kemija / *Chemistry* FMF – VS
Osnove kemije / *Fundamentals of Chemistry* FGG – UN
Splošna kemija / *General Chemistry* BF – UN
Anorganska kemija / *Inorganic Chemistry* FFA – UN
Splošna in anorganska kemija / *General and Inorganic Chemistry* FFA – UN
Splošna in organska kemija / *General and Organic Chemistry* FFA – UN
Anorganska kemija / *Inorganic Chemistry* NTF – VS
Osnove kemije / *Fundamentals of Chemistry* NTF – VS
Splošna in fizikalna kemija / *General and Physical Chemistry* BF – UN
Splošna kemija / *General Chemistry* PEF – UN
Anorganska kemija / *Inorganic Chemistry* PEF – UN

Predbolonjski dodiplomski programi / *Pre-Bologna Undergradutate Programmes*

Strukturna kemija / *Structural Chemistry* PEF – UN

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Kemija trdnega stanja / *Solid State Chemistry* – NTF

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

– Sinteze kovinskih karboksilatov in njihovih derivatov ter raziskave njihove uporabe kot zaščitnih premazov za les ter načina vezave kovinskih ionov na les. Sinteza in uporaba novih škorpijonatnih ligandov / *Syntheses of Metal Carboxylates and their Derivatives; Research into their Application as Protecting Layers for Wood and Type of Metal Ion Bonding in Wood. Synthesis and Application of New Scorpionate Ligands.*

- Kemija rutenijevih spojin. Sinteza, fizikalno-kemijska in biološka karakterizacija / *Chemistry of Ruthenium Compounds. Synthesis, Physico-Chemical and Biological Characterization.*
- Raziskave v kemiji kroma, molibdena in volframa: koordinacijske spojine in okso skupki / *Chemistry of Chromium, Molybdenum and Tungsten: Coordination Compounds and Oxo-Clusters*
- Sinteze novih brezvodnih lantanoidnih kompleksov iz oksidov / *Syntheses of Novel Anhydrous Lanthanoid Complexes from Oxides*
- Organokovinske spojine: raziskave novih organokovinskih fluoridov in njihove uporabe v katalizi / *Metal-Organic Compounds: Research into Novel Metal-Organic Fluorides and their Applications in Catalysis*
- Študij interakcij kovinskih ionov z biološko aktivnimi ligandi kinoloni in protiviralnimi nukleotidnimi analogi / *Studies of Interactions of Metal Ions with Biologically Active Quinolone Ligands and Anti-Viral Nucleotide Analogues*
- Rentgenska strukturna analiza monokristalov (koordinacijske in organske spojine) ter prahov (keramika) / *X-Ray Structure Analysis of Single Crystals (Coordination and Organic Compounds) and Powders (Ceramics)*
- Sol-gel priprava organsko-anorganskih hibridov z ionsko prevodnostjo / *Sol-Gel Preparation of Organic-Inorganic Hybrids Exhibiting Ionic Conductivity*
- Koordinacijske spojine platine, ki so potencialno uporabne kot citostatiki in virostatiki / *Coordination Compounds of Platinum, Potentially Applicable as Cytostatics and Virostatics*
- Vezava kovinskih ionov na biološke makromolekule, kot je npr. hialuronska kislina / *Bonding of Metal Ions on Biological Macromolecules, e.g. Hialuronic Acid*
- Imobilizacija kovinskih zvrsti v kontaminirani zemlji / *Immobilization of Metal Species in Contaminated Soil*
- Kemijska stabilizacija kovin v onesnaženih tleh in trdnih odpadkih / *Chemical Stabilization of Metals in Contaminated Soil and Solid Waste*
- Anaerobna razgradnja glukoze v prisotnosti cianida / *Anaerobic Degradation of Glucose in the Presence of Cyanide*
- Študij nanosa in strukture tankih plasti / *Studies on the Deposition of Thin Films*
- Razvoj ionskih hranilnikov / *Development of Ionic Containers*
- Termična analiza / *Thermal Analysis*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

- I. Turel, sourednik / *Co – Editor,* 2006–, *Metal-Based Drugs*, Hindawi Publishing Corporation
- I. Turel, regionalni urednik / *Regional Editor* of *"Molecules", A Journal of Synthetic Organic Chemistry and Natural Product Chemistry*
- P. Šegedin, sourednik / *Co-Editor, Acta Chimica Slovenica*
- I. Leban, član / *Member, Advisory Board, Macedonian Journal of Chemistry and Chemical Technology*

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

– I. Leban, sopredsednik organizacijskega odbora, N. Lah, A. Golobič, A. Meden, člani organizacijskega odbora 19. slovensko–hrvaškega srečanja kristalografov, Strunjan, Slovenija, junij 2010 / *Co-Chairman and Members of the Organisig Committee of the 19th Slovenian-Croatian Crystallographic Meeting, Strunjan, Slovenia, June 2010*

DRUGO / OTHER

– I. Leban, strokovnjak v Institutional Evaluation Programme Evropskega združenja univerz (EUA) / *Expert in the Institutional Evaluation Programme, European Universities Association*
– I. Leban, »Noč raziskovalcev 2010«, eksperimentalno predavanje za popularizacijo kemije / *»Researchers' Night 2010« – Demonstration Lecture for the Popularization of Chemistry*
– I. Leban, član nacionalne komisije (kot predstavnik UL FKKT) za organizacijo dogodkov v Mednarodnem letu kemije (IYC) 2011 / *Member of the National Committee for the Organisation of Events in the International Year of Chemistry (IYC 2011)*
– S. Petriček, predsednica Državne predmetne komisije za splošno maturo iz kemije / *Chairman of the Subject Testing Committee for the Matura in Chemistry*
– F. Perdih, mentor znanstvene ekipe študentov FKKT na XIV. mednarodnem znanstveno-športnem srečanju – Tehnologijada 2010, Šibenik, Hrvaška, april 2010 / *Mentor of the FKKT Students Scientific Team at the XIV. International Scientific and Sports Meeting – Tehnologijada 2010, Šibenik, Croatia, April 2010*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

– Modularni sistem za termično analizo – Mettler Toledo (TGA/SDTA 851, DSC 822, HP DSC 827 + modul za termoluminiscenco s kamero PRO. sensicam) / *Modular System for Thermal Analysis – Mettler Toledo (TGA/SDTA 851, DSC 822, HP DSC 827 + Module for Thermoluminescence with PRO. sensicam)*
– Modularni sistem za termično analizo – Mettler Toledo (TGA/DSC 1 + modul za TGA/FTIR / *Modular System for Thermal Analysis Mettler Toledo (TGA/DSC 1 + Module for TGA/FTIR*
– Modularni sistem za termično analizo – Perkin Elmer (TGA7, DTA7) / *Modular System for Thermal Analysis – Perkin Elmer*
– HPLC kromatograf / *HPLC Chromatograph*
– Polarizacijski mikroskop / *Polarisation Microscope*
– Stereomikroskop / *Stereomicroscope*
– Difraktometer za monokristale Nonius Enraf CAD 4 / *Single-Crystal Diffractometer Nonius Enraf CAD 4*
– Difraktometer za monokristale Nonius Kappa CCD + kriostat za tekoči dušik Oxford Cryosystem 700 / *Single-Crystal Diffractometer Nonius Kappa CCD + Oxford Cryosystem 700 for Liquid Nitrogen*
– Visoko ločljivi rentgenski praškovni difraktometer s $CuK_{\alpha 1}$ radiacijo (50 % solastništvo s Kemijskim inštitutom / *High Resolution X-ray Powder Diffractometer (Shared with the National Institute of Chemistry)*

- Spektrometer Perkin Elmer SPECTRUM 100 / *Perkin Elmer* SPECTRUM 100 *Spectrometer*
- ATR Specac Golden Gate / *ATR Specac Golden Gate*
- Spektrometer Perkin Elmer Lambda 750 / *Perkin Elmer Lambda 750 Spectrometer*
- Spektrometer Perkin Elmer UV/VIS/NIR Lambda 19 / *Perkin Elmer UV/VIS/NIR Lambda 19 Spectrometer*
- Fluorimeter Perkin Elmer LS 55 / *Perkin Elmer Fluorescence Spectrometer LS 55*
- Magnetna tehtnica AVTO, Sherwood Scientific */ Magnetic Susceptibility Balance AVTO, Sherwood Scientific*
- Suha komora MBraun Unilab */ Dry Box MBraun Unilab*
- Planetarni mlin PM100 Retsch / *Planetary Mill PM100 Retsch*
- OxiTop WTW */ OxiTop WTW*
- Spektrometer Varian *Carry 50* z zunanjo optično sondo / *Spectrometer Varian Carry 50 with Optical Probe*

SODELOVANJE V CENTRIH ODLIČNOSTI / CENTERS OF EXCELLENCE

Center odličnosti: CO NOT – Nizkoogljične tehnologije / *Center of Excellence: Low-Carbon Technologies*

Center odličnosti: EN-FIST – raziskave na področju zdravja, znanosti o življenju in naprednih novih materialov / *Center of Excellence: Multidisciplinary Research in Life Sciences and Advanced New Materials*

Center odličnosti: CO NAMASTE – Napredni nekovinski materiali in tehnologije prihodnosti / *Center of Excellence: Advanced Materials and Technologies for the Future*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P1–0134	Bioanorganska in bioorganska kemija / *Bioinorganic and Bioorganic Chemistry* Vodja programa / *Principal Researcher*: P. Bukovec
P1–0175	Sinteza, struktura, lastnosti snovi in materialov / *Synthesis, Structure and Properties of Compounds and Materials* Vodja programa / *Principal Researcher*: I. Leban

TEMELJNI PROJEKTI / BASIC RESEARCH

J1–0200	Sinteza novih protitumorskih rutenijevih spojin / *Synthesis of Novel Antitumor Ruthenium Compounds* Nosilec / *Principal Researcher*: I. Turel

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L2–1129	Razvoj fotokatalitskih prevlek in plinskih fotoreaktorjev / *Development of Photocatalytic Coatings and Gas Photoreactors* Nosilec / *Principal Researcher*: P. Bukovec Sofinancer / *Co-sponsored by*: Martex d.o.o.
L4–2144	Premazi iz utekočinjenega lesa / *Liquified Wood Coatings* Nosilec / *Principal Researcher*: P. Bukovec Sofinancer / *Co-sponsored by*: Tanin Sevnica d.d.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI V RS / COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS IN SLOVENIA

- Krka d.d.: Ekspertne storitve (letna pogodba) / *Expert Services (Annual Contract)*
- UNICHEM d.o.o.: Razvoj biocidnih sredstev in gnojil (pogodba KPIOT) / *Development of Biocidal Agents and Fertilizers*

RAZISKOVALNI PROJEKTI (DRUGI NAROČNIKI) / RESEARCH PROJECTS (OTHER CONTRACTORS)

ESS (Evropski socialni sklad –projekti / *European Social Fund*	Razvoj naravoslovnih kompetenc / *Development of Competences in Natural Sciences* Nosilec projekta / *Project Leader*: UM Fakulteta za naravoslovje in matematiko / *University of Maribor, Faculty of Natural Science and Mathematics* FKKT partner v projektu / *FKKT Project Partner* Koordinatorka partnerskih fakultet / *Partnership Coordinator of Faculties*: N. Bukovec

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

COST D39	*Metallo-Drug Design and Action* Nosilka / *Principal Researcher*: S. Grabner
COST 540	*Photocatalytic Technologies and Novel Nanosurface Materials* Članica upravnega odbora / *Steering Committe Member*: R. Cerc Korošec
COST D39	*Ruthenium Anticancer Compounds* Nosilec / *Principal Researcher*: I. Turel

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Avstrija *Slovenia – Austria*	Rutenijeve spojine in njihova možna uporaba v elektrokemoterapiji / *Ruthenium Compounds and their*

	Possible Applications in Electrochemotherapy Nosilec / *Principal Researcher*: I. Turel
Slovenija – Češka republika *Slovenia – Czech Republic*	Reakcije fosfatov in fosfonatov z organotitanovimi(IV) fluoridi in alkoksidi / *Reactions of Phosphates and Phosphonates with Organotitanium(IV) Fluorides and Alkoxides* Nosilec / *Principal Researcher*: A. Pevec

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

AK1. JUG, Aleš, PETELIN, Stojan, BUKOVEC, Peter. Designing an underground car park fire scenarios on a probabilistic basis. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 136–143. [COBISS.SI-ID 33809157]

AK2. KASUNIČ, Marta, GAČNIK, Ksenija, ŠEGEDIN, Primož, GOLOBIČ, Amalija. Preparation, characterization and crystal structure of [Cu[sub]2(O[sub]2CH)[sub]4(nicotinamide)[sub]2]. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 2, str. 350–354. [COBISS.SI-ID 34167045]

AK3. PETRIČEK, Saša, DEMŠAR, Alojz. Syntheses and crystal structures of manganese, nickel and zinc chloride complexes with dimethoxyethane and di(2-methoxyethyl) ether. Polyhedron. [Print ed.], 2010, vol. 29, no. 18, str. 3329–3334, doi: 10.1016/j.poly.2010.09.014. [COBISS.SI-ID 34687493]

AK4. BARCELÓ-OLIVER, Miquel, TERRÓN, Angel, GARCÍA-RASO, Angel, LAH, Nina, TUREL, Iztok. Intermolecular C-H[times][times][times][pi] interactions in 1,5-diphenyl-3-(2-pyridyl)-2-pyrazoline. *Acta crystallogr., C Cryst. struct. commun.*, 2010, vol. C66, no. 6, str. 313–316. [COBISS.SI-ID 34080261]

AK5. HUDEJ, Rosana, TUREL, Iztok, KANDUŠER, Maša, ŠČANČAR, Janez, KRANJC, Simona, SERŠA, Gregor, MIKLAVČIČ, Damijan, JAKUPEC, Michael, KEPPLER, Bernhard K., ČEMAŽAR, Maja. The influence of electroporation on cytotoxicity of anticancer ruthenium(III) complex KP1339 in vitro and in vivo. *Anticancer res.*, 2010, vol. 30, no. 6, str. 2055–2063. [COBISS.SI-ID 34301957]

AK6. KLJUN, Jakob, PETRIČEK, Saša, ŽIGON, Dušan, HUDEJ, Rosana, MIKLAVČIČ, Damijan, TUREL, Iztok. Synthesis and characterization of novel ruthenium(III) complexes with histamine. *Bioinorganic chemistry and applications*. [Online ed.], 2010, str. 1–6. [COBISS.SI-ID 34117893]

AK7. MALI, Gregor, MEDEN, Anton, DOMINKO, Robert. [sup] 6 Li MAS NMR spectroscopy and first-principles calculations as a combined tool for the investigation of Li [sub] 2 MnSiO [sub] 4 polymorphs. *Chem. commun. (Lond., 1996)*, 2010, issue 19, str. 3306–8. [COBISS.SI-ID 4386074]

AK8. SEPČIĆ, Juraj, BUČUK, Mira, PERKOVIĆ, Olivio, ŠEPIĆ-GRAHOVAC, Dubravka, TROŠELJ VUKIĆ, Biserka, POLJAK, Ivica, CRNIĆ-MARTINOVIĆ, Marija, TUREL, Iztok, RISTIĆ, Smiljana, SEPČIĆ, Kristina. Drug-induced aseptic meningitis, sensorineural hearing loss and vestibulopaty. *Coll. antropol.*, 2010, vol. 34, no. 3, str. 1101–1104. [COBISS.SI-ID 2281295]

AK9. URANKAR, Damijana, PEVEC, Andrej, TUREL, Iztok, KOŠMRLJ, Janez. Pyridyl conjugated 1,2,3-triazole is a versatile coordination ability ligand enabling supramolecular associations. *Cryst. growth des.*, 2010, vol. 10, no. 11, str. 4920–4927. [COBISS.SI-ID 34469381]

AK10. KASTELIC, Jože, HODNIK, Žiga, ŠKET, Primož, PLAVEC, Janez, LAH, Nina, LEBAN, Ivan, PAJK, Matjaž, PLANINŠEK, Odon, KIKELJ, Danijel. Fluconazole cocrystals with dicarboxylic acids. *Cryst. growth des.*, 2010, vol. 10, no. 11, str. 4943–4953. [COBISS.SI-ID 2881905]

AK11. MARQUÉS-GALLEGO, Patricia, GAMIZ-GONZALES, M. Amparo, FORTEA-PÉREZ, Francisco R., LUTZ, Martin, SPEK, Anthony L., PEVEC, Andrej, KOZLEVČAR, Bojan, REEDIJK, Jan. Quinoxaline-2-carboxamide as a carrier ligand in two new platinum(II) compounds : synthesis, crystal structure, cytotoxic activity and DNA interaction. *Dalton trans. (2003. Print)*, 2010, vol. 39, no. 21, str. 5152–5158. [COBISS.SI-ID 34101253]

AK12. MOOIBROEK, Tiddo Jonathan, GAMEZ, Patrick, PEVEC, Andrej, KASUNIČ, Marta, KOZLEVČAR, Bojan, FU, Wen-Tian, REEDIJK, Jan. Efficient, stable, tunable, and easy to synthesize, handle and recycle luminescent materials : [H[sub]2NMe[sub]2][sub]3[Ln(III)(2, 6-dipicolinolate)[sub]3] (Ln = Eu, Tb, or its solid solutions). *Dalton trans. (2003. Print)*, 2010, vol. 39, no. 28, str. 6483–6847. [COBISS.SI-ID 34476037]

AK13. MODEC, Barbara, ŠALA, Martin, CLÉRAC, Rodolphe. Pyrazine-assisted dimerization of molybdenum(V) : synthesis and structural characterization of novel dinuclear and tetranuclear complexes. *European Journal of Inorganic Chemistry*, 2010, no. 4, str. 542–553. [COBISS.SI-ID 33587973]

AK14. ŠTEFANE, Bogdan, PERDIH, Andrej, PEVEC, Andrej, ŠOLMAJER, Tomaž, KOČEVAR, Marijan. The participation of 2H-pyran-2-ones in [4+2] cycloadditions : an experimental and computational study. *European journal of organic chemistry*, 2010, vol. 2010, issue 30, str. 5870–5883. [COBISS.SI-ID 34399749]

AK15. URANKAR, Damijana, PINTER, Balazs, PEVEC, Andrej, DE PROFT, Frank, TUREL, Iztok, KOŠMRLJ, Janez. Click-triazole N2 coordination to transition-metal ions is assisted by a pendant pyridine substituent. *Inorg. chem.*, 2010, vol. 49, no. 11, str. 4820–4829. [COBISS.SI-ID 34066949]

AK16. TUREL, Iztok, KLJUN, Jakob, PERDIH, Franc, MOROZOVA, Elena, BAKULEV, Vladimir, KASYANENKO, Nina, BYL, Jo Ann W., OSHEROFF, Neil. First ruthenium organometallic complex of antibacterial agent ofloxacin. Crystal structure and interactions with DNA. *Inorg. chem.*, 2010, vol. 49, no. 23, str. 10750–10752. [COBISS. SI-ID 34623493]

AK17. DOJER, Brina, PEVEC, Andrej, ŠEGEDIN, Primož, JAGLIČIĆ, Zvonko, STROPNIK, Črtomir, KRISTL, Matjaž, DROFENIK, Mihael. Cobalt(II) coordination compounds with acetato and 2-aminopyridine ligands: Synthesis, characterisation, structures and magnetic properties of two polymorphic forms. *Inorg. Chim. Acta*. [Print ed.], 2010, issue 7, vol.363, str. 1343–1347. [COBISS.SI-ID 13809942]

AK18. CEFALAS, Alciviadis-Constantinos, SARANTOPOULOU, Evangelia, KOLLIA, Zoe, RIZIOTIS, C., DRAŽIĆ, Goran, KOBE, Spomenka, STRAŽIŠAR, Janez, MEDEN, Anton. Magnetic field trapping in coherent antisymmetric states of liquid water molecular rotors. *j. comput. theor. nanosci.*, 2010, vol. 7, no. 9, str. 1800–1805. [COBISS.SI-ID 23692583]

AK19. KRISTL, Matjaž, DOJER, Brina, KASUNIČ, Marta, GOLOBIČ, Amalija, JAGLIČIĆ, Zvonko, DROFENIK, Mihael. Hydroxylammonium fluorometalates : synthesis and characterisation of a new fluorocuprate and fluorocobaltate. *J. fluorine chem.*. [Print ed.], Sep. 2010, vol. 131, iss. 9, str. 907–914. [COBISS.SI-ID 14192662]

AK20. POPOV-PERGAL, K., POLETI, Dejan, RANČIĆ, M., MEDEN, Anton, PERGAL, Marija V. Synthesis and structure of new 5-(arylidene)-3-(4-methylbenzoyl)thiazolidine-2,4-diones. *J. heterocycl. chem.*, 2010, vol. 47, no. 1, str. 224–228. [COBISS.SI-ID 33969925]

AK21. SKYRIANOU, Kalliopi C., PERDIH, Franc, TUREL, Iztok, KESSISSOGLOU, Dimitris P., PSOMAS, George. Nickel-quinolones interaction. Part 2, Interaction of nickel(II) with the antibacterial drug oxolinic acid. *J. inorg. biochem.*. [Print ed.], 2010, vol. 104, no. 2, str. 161–170. [COBISS.SI-ID 33541125]

AK22. SKYRIANOU, Kalliopi C., PERDIH, Franc, TUREL, Iztok, KESSISSOGLOU, Dimitris P., PSOMAS, George. Nickel-quinolones interaction. Part 3, Nickel(II) complexes of the antibacterial drug flumequine. *J. inorg. biochem.*. [Print ed.], 2010, vol. 104, no. 7, str. 740–749. [COBISS.SI-ID 34055941]

AK23. ZABUKOVEC LOGAR, Nataša, MALI, Gregor, RAJIĆ, Nevenka, JEVTIĆ, Sanja, RANGUS, Mojca, GOLOBIČ, Amalija, KAUČIČ, Venčeslav. Structure investigation of fluuorinated aluminophosphate ULM-3 Al templated by 3-methylaminopropylamine. *J. solid state chem.*, 2010, issue 5, vol. 183, str. 1055–1062. [COBISS.SI-ID 4385562]

AK24. VEBER, Asja, KUNEJ, Špela, CERC KOROŠEC, Romana, SUVOROV, Danilo. The effects of solvents on the formation of sol-gel-derived Bi[sub](12)SiO[sub](20) thin films. *J. Eur. Ceram. Soc.*. [Print ed.], 2010, vol. 30, no. 12, str. 2475–2480. [COBISS.SI-ID 23796263]

AK25. ANTIĆ, Bratislav, KREMENOVIĆ, Aleksandar, VUČINIĆ-VASIĆ, Milica, DOHČEVIĆ-MITROVIĆ, Zorana D., NIKOLIĆ, A. S., GRUDEN-PAVLOVIĆ, M., JANČAR, Boštjan, MEDEN, Anton. Composition related properties of (Yb,Y)[sub]2O[sub]3 nanoparticles synthesized by controlled thermal degradation of AA complexes. *Mater. chem. phys.*. [Print ed.], 2010, issue 2–3, vol.122, str. 386–391. [COBISS.SI-ID 33970437]

AK26. TRATAR-PIRC, Elizabeta, LEVSTEK, Meta, BUKOVEC, Peter. Influence of cyanide on the anaerobic degradation of glucose. Water sci. technol., 2010, vol. 62, no. 8, str. 1799–1806, doi: 10.2166/wst.2010.467. [COBISS. SI-ID 34752005]

AK27. MODEC, Barbara, ZUBIETA, Jon. Syntheses and a solid state structure of a dinuclear molybdenum(V) complex with pyridine. *Materials (Basel)*, 2010, vol. 3, no. 1, str. 150–157. [COBISS.SI-ID 33588997]

AK28. OMERZU, Aleš, ANŽELAK, Bernarda, TUREL, Iztok, ŠTRANCAR, Janez, POTOČNIK, Anton, ARČON, Denis, ARČON, Iztok, MIHAILOVIĆ, Dragan, MATSUI, Hiroshi. Strong correlations in highly electron-doped Zn(II)-DNA complexes. *Phys. rev. lett.*, 16. apr. 2010, vol. 104, no. 15, str. 156804-1-156804-4. [COBISS.SI-ID 1459451]

AK29. NAYAK, Sanjit, GAMEZ, Patrick, KOZLEVČAR, Bojan, PEVEC, Andrej, ROUBEAU, Oliver, DEHNEN, Stefanie, REEDIJK, Jan. Coordination compounds from the planar tridentate Schiff-base ligand 2-methoxy-6--((quinolin-8-ylimino)methyl)phenol (mqmpH) with several transition metal ions : use of [Fe[sup]III(mq,p)(CH[sub]3OH)Cl[sub]2] in the catalytic oxidation of alkanes and alkenes. *Polyhedron*. [Print ed.], 2010, issue 11, vol. 29, str. 2291–2296. [COBISS.SI-ID 34101765]

AK30. ĐAKOVIĆ, Marijana, JAGLIČIĆ, Zvonko, KOZLEVČAR, Bojan, POPOVIĆ, Zora. Association of copper(II) isonicotinamide moieties via different anionic bridging ligands : two paths of ferromagnetic interaction in the azide coordination compound. *Polyhedron*. [Print ed.], 2010, vol. 29, no. 8, str. 1910–1919. [COBISS.SI-ID 34010629]

AK31. KOZJEK-ŠKOFIC, Irena, PADEŽNIK GOMILŠEK, Jana, KODRE, Alojz, BUKOVEC, Nataša. Electrochemical, optical and X-ray absorption studies of Ce/V mixed oxides thin films. *Sol. energy mater. sol. cells*. [Print ed.], 2010, vol. 94, no. 3, str. 554–559. [COBISS.SI-ID 33658117]

AK32. LAH, Nina, LEBAN, Ivan. Three new copper(II) halides with simple pyridine alcohols. *Struct. chem.*, 2010, vol. 21, no. 1, str. 263–267. [COBISS.SI-ID 33686789]

AK33. ŽEROVNIK, Darja, GROŠELJ, Uroš, KRALJ, David, MALAVAŠIČ, Črt, BEZENŠEK, Jure, DAHMANN, Georg, STARE, Katarina, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Synthesis of 1,5,6,7-tetrahydro-4H-pyrazolo[4,3-c]pyridin-4-ones as conformationally constrained pyrazole analogues of histamine. *Synthesis (Stuttg.)*, 2010, no. 19, str. 3363–3372. [COBISS.SI-ID 34495237]

AK34. BEZENŠEK, Jure, KOLEŠA, Tanja, GROŠELJ, Uroš, WAGGER, Jernej, STARE, Katarina, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. [2+2] Cycloaddition of electron-poor acetylenes to (E)-3-dimethylami-

no-1-heteroaryl-prop-2-en-1-ones : synthesis of highly functionalized 1-heteroaroyl-1,3-butadienes. *Tetrahedron lett.*. [Print ed.], 2010, vol. 51, no. 26, str. 3392–3397. [COBISS.SI-ID 34086917]

AK35. LONCNAR, Mojca, ZUPANČIČ, Marija, BUKOVEC, Peter, ZUPANČIČ JUSTIN, Maja. Fate of saline ions in a planted landfill site with leachate recirculation. *Waste manag. (Elmsford)*. [Print ed.], 2010, vol. 30, no. 1, str. 110–118. [COBISS.SI-ID 33263365]

AK36. ZUPANČIČ JUSTIN, Maja, PAJK, Nastja, ZUPANC, Vesna, ZUPANČIČ, Marija. Phytoremediation of landfill leachate and compost wastewater by irrigation of Populus and Salix : Biomass and growth response. *Waste manag. (Elmsford)*. [Print ed.], 2010, letn. 30, str. 1032–1042. [COBISS.SI-ID 26762969]

AK37. ŠIMUNEK, P., BAŠKOVČ, Jernej, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. The structure of the product formed by condensation of malononitrile with dialkyl acetone-1,3-dicarboxylates. *Z. Nat.forsch., B J. chem. sci.*, 2010, vol. 65b, no. 6, str. 807–810. [COBISS.SI-ID 34205957]

AK38. COSTA, José Sánchez, GONZALES CASTRO, Adriana, PIEVO, Roberta, ROUBEAU, Olivier, MODEC, Barbara, KOZLEVČAR, Bojan, TEAT, S. J., GAMEZ, Patrick, REEDIJK, Jan. Proficiency of the electron-deficient 1,3,5-triazine ring to generate anion-[pi] and ione pair-[pi] interactions. *CrystEngComm (Camb., Online)*, 2010, vol. 12, no. 10, str. 3057–3064. [COBISS.SI-ID 34667269]

AK39. ÖZALP-YAMAN, Şeniz, HOOG, Paul de, MAHESWARI, Palanisamy Uma, CASELLAS, Hélène, GOLOBIČ, Amalija, KOZLEVČAR, Bojan, GAMEZ, Patrick, REEDIJK, Jan. Spectroelectrochemical studies of nuclease--active zinc(II) coordination compounds from the ligands Hpyramol and Hpyrimol. *Electrochim. acta*. [Print ed.], 2010, vol. 55, no. 28, str. 8655–8663. [COBISS.SI-ID 34668037]

AK40. UMEK, Polona, CERC KOROŠEC, Romana, GLOTER, Alexandre, PIRNAT, Urša. The control of the diameter and length of [alpha]-MnO[sub]2 nanorods by regulation of reaction parameters and their thermogravimetric properties. *Mater. res. bull.*. [Print ed.], [in press] 2010, 8 str.[COBISS.SI-ID 24111399]

KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

AK41. KASUNIČ, Marta, VERČEK, Bojan, MUŠIČ, Irena, GOLOBIČ, Amalija. 3-Benzamido-1-benzoyl-1H-pyrrol--2(5H)-one. *Acta crystallographica. E, Structure Reports*, 2010, vol. E66, no. 3, str. o687 (6 str. suppl.). [COBISS.SI-ID 33745413]

AK42. BARCELÓ-OLIVER, Miquel, TERRÓN, Angel, GARCÍA-RASO, Angel, TUREL, Iztok, MORELL, Marta. Di-[mu]-chlorido-bis{chlorido[(R)/(S)-1, 5-diphenyl-3-(2-pyridyl-[kappa]N)-2 -pyrazoline-[kappa]N[sup]2] zinc(II)}. *Acta crystallographica. E, Structure Reports*, 2010, vol. E66, no. 8, str. m899-m900 (11 str. suppl.). [COBISS.SI-ID 34196485]

AK43. GENORIO, Boštjan, PIRNAT, Klemen, CERC KOROŠEC, Romana, DOMINKO, Robert, GABERŠČEK, Miran. Electroactive organic molecules immobilized onto solid nanoparticles as a cathode material for lithium-ion batteries. *Angew. Chem. (Int. ed., Print)*. [Print ed.], 2010, vol. 49, no. 40, str. 7222–7224. [COBISS.SI-ID 34436869]

AK44. GOLOBIČ, Amalija, ČEH, Boris. [mu]-Oxido-bis{[2,2-bis(3,5-dimethyl-1H-pyrazol-yl)acetato-[kappa][sup]3N [s up]2,O, N[sup]2']chloridooxidomolybdenum(V)} monohydrate. Acta crystallographica. E, Structure Reports, 2010, vol. E66, no. 12, str. m1648-m1649, [COBISS.SI-ID 34680325]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

AK45. ŽGAJNAR GOTVAJN, Andreja, KALČÍKOVÁ, Gabriela, ZUPANČIČ, Marija, ZAGORC-KONČAN, Jana. Determination of inhibitory effects of landfill leachate on nitrification. V: *Book of Abstracts of the Second International Symposium on Green Chemistry for Environment and Health : Mykonos, Royal Mykonian Hotel & Thalasso Spa, September 26–29, 2010 : Elektronski vir*. Thessaloniki: Grafima, 2010, str. [1–6]. [COBISS.SI-ID 34505477]

AK46. TRATAR-PIRC, Elizabeta. Anaerobic degradation of glucose in presence of cyanide. V: Protection and Restoration of the Environment X, 5–9 July 2010, Corfu, Greece. *Conference proceedings : Pre10*. [S. l.: s. n.], 2010, str. [1–8]. [COBISS.SI-ID 34231557]

AK47. TRATAR-PIRC, Elizabeta, ŠAUTA OGOREVC, Jerneja, BUKOVEC, Peter. Anaerobic degradation of Plasmocorinth B in comparison to photodegradation with TiO2 thin films. V: Protection and Restoration of the Environment X, 5–9 July 2010, Corfu, Greece. *Conference proceedings : Pre10*. [S. l.: s. n.], 2010, str. [1–8]. [COBISS.SI-ID 34231813]

AK48. ZUPANČIČ, Marija, CENCELJ, Jure, BUKOVEC, Peter. Evaluation of the use of phosphate stabilisation agents for metal contaminated soils. V: Protection and Restoration of the Environment X, 5–9 July 2010, Corfu, Greece. *Conference proceedings : Pre10*. [S. l.: s. n.], 2010, str. [1–8]. [COBISS.SI-ID 34277125]

AK49. CERC KOROŠEC, Romana, REP, Gregor, POHLEVEN, Franc, BUKOVEC, Peter. Thermogravimetrical analysis of heat treated spruce wood – a possible tool for external quality control?. V: HILL, Callum A. S. (ur.), MILITZ, Holger (ur.), ANDERSONS, Bruno (ur.). *The fifth European conference on wood modification : ECWM5, September 20–21, 2010 Riga, Latvia : proceedings*. Riga: Latvian State Institute of Wood Chemistry, 2010, str. 259–262. [COBISS.SI-ID 1835913]

AK50. ZUPANČIČ, Marija, BUKOVEC, Peter. Evaluation of the metal stabilization efficiency and drawbacks of phosphate treatment of contaminated soil. V: BARGAŃSKA, Żaneta (ur.). *Proceedings of the 15th International Conference on Heavy Metals in the Environment, September 19–23, 2010, Gdańsk, Poland*. Gdańsk: Chemical Faculty, Gdańsk University of Technology, 2010, str. 486–489. [COBISS.SI-ID 34481925]

AK51. LONCNAR, Mojca, ZUPANČIČ, Marija, BUKOVEC, Peter, JAKLIČ, Anton. Hot stage processing of slag and its leaching characteristics. V: BARGAŃSKA, Żaneta (ur.). *Proceedings of the 15th International Conference on Heavy Metals in the Environment, September 19–23, 2010, Gdańsk, Poland*. Gdańsk: Chemical Faculty, Gdańsk University of Technology, 2010, str. 1006–1009. [COBISS.SI-ID 34482181]

AK52. MAKAROVIČ, Kostja, MEDEN, Anton, HROVAT, Marko, BELAVIČ, Darko, HOLC, Janez. Influence of processing conditions on the characteristics of LTCC materials. V: ESTC 2010, Electronics System Integration Technology Conference, September 13–16 2010, Berlin, Germany. *Proceedings*. [S. l.: s. n.], 2010, 4 str. [COBISS.SI-ID 23947559]

AK53. JUG, Aleš, PETELIN, Stojan, BUKOVEC, Peter. Correlation of underground car park impulse ventilation control and realistic fire scenarios. V: ANŽEK, Mario (ur.), HERNAVS, Boštjan (ur.), KAVRAN, Zoran (ur.), MEŠE, Pavel (ur.), ŠTERN, Andrej (ur.). 18th International Symposium on Electronics in Traffic, ISEP 2010, March 29, 2010, Ljubljana. *The role of ITS in the near future : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2010, f. [1–7]. [COBISS.SI-ID 33865221]

AK54. KOZLEVČAR, Bojan. Bakrove(II) koordinacijske spojine z gvajacilnimi (4-hidroksi-3-metoksifenil) ligandi = Copper(II) coordination compounds with guaiacyl (4-hydroxy-3-methoxyphenyl) ligands. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–5. [COBISS.SI-ID 34459653]

AK55. BEZENŠEK, Jure, KOLEŠA, Tanja, GROŠELJ, Uroš, WAGGER, Jernej, STARE, Katarina, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. [2+2] Cikloadicije elektronsko revnih acetilenov na »push-pull« dimetilaminopropenoate = [2+2] Cycloadditions of electron-poor acetylenes on push-pull dimethylaminopropenoates. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–7. [COBISS.SI-ID 34459397]

AK56. PERDIH, Franc. Strukture [Cp*[spodaj]2Ti[spodaj]2F[spodaj]7][na]- in [Cp*[spodaj]2ti[spodaj]2F[spodaj]3(SO[spodaj]4)[spodaj]2][na]- anionov = Structures of [Cp*[sub]2Ti[sub]2F[sub]7][sup]- and [Cp*[sub]2Ti[sub]2F[sub]3(SO[sub]4)[sub]2][sup]- anions. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–7. [COBISS.SI-ID 34459909]

AK57. TRATAR-PIRC, Elizabeta. Sestava bioplina pri anaerobni razgradnji glukoze v prisotnosti cianidov = Biogas composition at anaerobic degradation of glucose in presence of cyanide. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–8. [COBISS.SI-ID 34468613]

AK58. KRANJC, Krištof, PERDIH, Franc, KOČEVAR, Marijan. Vpliv velikosti obroča na ekso/endo selektivnost pri dvojni termični Diels-Alderjevi reakciji pripojenih piran-2-onov = Effects of ring size on the exo/endo selectivity of a thermal double Diels-Alder reaction of fused pyran-2-ones. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–8. [COBISS.SI-ID 34459141]

AK59. MALAVAŠIČ, Črt, WAGGER, Jernej, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Priprava, struktura in uporabnost kiralnih N-alkiliranih cikličnih dipeptidov = Preparation, structure and applicability of chiral N-alkylated cyclic dipeptides. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–9. [COBISS.SI-ID 34449413]

AK60. CER KERČMAR, Ksenija, TRATAR-PIRC, Elizabeta, MODEC, Barbara, BUKOVEC, Peter. Sinteza in karakterizacija bakrovega(II) kompleksa s ksanturinsko kislino = Synthesis and characterization of copper(II) complex with xanthurenic acid. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–10. [COBISS.SI-ID 34460165]

AK61. NOGRAŠEK, Boštjan, KOZLEVČAR, Bojan, GOLOB, Janvit, LIKOZAR, Blaž. Načrtovanje integriranega procesa oplaščanja zrn umetnih gnojil in sušenja v fluidiziranem sloju = Design of integrated process of synthetic fertilizer coating process and drying in fluidized bed. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–11. [COBISS.SI-ID 34477061]

AK62. KITANOVSKI, Nives. Spojine s polipirazolil škorpionatnimi ligandi = Compounds with polypyrazolyl scorpionate ligands. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–15. [COBISS.SI-ID 34460421]

AK63. MAKAROVIČ, Kostja, MEDEN, Anton, HROVAT, Marko, KOSEC, Marija, BELAVIČ, Darko, HOLC, Janez. The structural development of LTCC materials during processing. V: BENČAN, Andreja (ur.), KUŠČER, Danjela (ur.), MALIČ, Barbara (ur.), KOSEC, Marija (ur.). *Workshop on structural characterisation : Jožef Stefan Institute, Ljubljana, Slovenia, 28 January 2010 : [program and abstract book]*. Ljubljana: Institut Jožef Stefan, Electronic Ceramic Department, 2010, str. 22. [COBISS.SI-ID 23387431]

OBJAVLJENI POVZETEK ZNANSTVENEGA PRISPEVKA NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION ABSTRACT (INVITED LECTURE)

AK64. TUREL, Iztok. Quinolone antibacterial agents and metal ions – friends or enemies? : [invited lecture]. V: 10th European Biological Inorganic Chemistry Conference, June 22–26, 2010, Thessaloniki, Greece. *Abstracts : authors' index*. [S. l.: s. n.], 2010, str. [1]. [COBISS.SI-ID 34198277]

AK65. MEDEN, Anton. X-ray powder diffraction analysis : (for structural characterization of ceramics) : [invited lecture]. V: BENČAN, Andreja (ur.), KUŠČER, Danjela (ur.), MALIČ, Barbara (ur.), KOSEC, Marija (ur.). *Workshop on structural characterisation : Jožef Stefan Institute, Ljubljana, Slovenia, 28 January 2010 : [program and abstract book]*. Ljubljana: Institut Jožef Stefan, Electronic Ceramic Department, 2010, str. 10. [COBISS.SI-ID 34085893]

SAMOSTOJNI ZNANSTVENI SESTAVEK ALI POGLAVJE V MONOGRAFSKI PUBLIKACIJI / INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

AK66. CERC KOROŠEC, Romana, BUKOVEC, Peter. Optimisation of the thermal-treatment of chemically prepared electrochromic nickel oxide thin films, their electrochromic properties and structural investigations. V: SOMANI, Prakash R. (ur.). *Chromic materials, phenomena and their technological applications*, (Multifunctional materials and devices). Pune: Applied Science Innovations Private Limited, 2010, str. 241–282. [COBISS.SI-ID 34674437]

UNIVERZITETNI ALI VISOKOŠOLSKI UČBENIK Z RECENZIJO / REVIEWED UNIVERSITY AND ACADEMIC TEXTBOOK

AK67. PETRIČEK, Saša, PERDIH, Franc, DEMŠAR, Alojz. *Vaje iz anorganske kemije za visokošolski strokovni študij kemijske tehnologije*. 3. dopolnjena izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 120 str., ilustr. ISBN 978-961-6756-19-8. [COBISS.SI-ID 252533760]

AK68. TUREL, Iztok, ZUPANČIČ, Marija. *Vaje iz splošne kemije*. 1. izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 72 str., ilustr. ISBN 978-961-6756-16-7. [COBISS.SI-ID 251562240]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

AK69. GLAŽAR, Saša A., GRAUNAR, Mojca, MODEC, Barbara, ŠKET, Barbara, ŠKET, Boris. *Kemija danes : učenje z nalogami : zbirka nalog za 8. in 9. razred devetletne osnovne šole*, (Raziskovalec 8), (Raziskovalec 9). 1. izd. Ljubljana: DZS, 2010. 184 str., ilustr. ISBN 978-86-341-3645-6. [COBISS.SI-ID 249326336]

AK70. BUKOVEC, Nataša, CERC KOROŠEC, Romana, TRATAR-PIRC, Elizabeta. *Praktikum iz splošne in anorganske kemije*. 2. dopolnjena izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 114 str., ilustr. ISBN 978-961-6756-18-1. [COBISS.SI-ID 252396544]

AK71. MODEC, Barbara. *Zbirka poskusov iz anorganske kemije za študente Pedagoške fakultete*. 1. izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 88 str., ilustr. ISBN 978-961-6756-14-3. [COBISS.SI-ID 251041792]

AK72. MEDEN, Anton, GOLOBIČ, Amalija. *Zgradba in lastnosti trdnin – vaje*. 1. izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 72 str., ilustr. ISBN 978-961-6756-12-9. [COBISS.SI-ID 249815552]

AK73. ČEH, Boris, DOLENC, Darko. Snovi, okolje, prehrana : učbenik za kemijo v srednjih strokovnih šolah. 1. izd. Ljubljana: DZS, 2010. 168 str., ilustr. ISBN 978-961-02-0077-2. [COBISS.SI-ID 252735232]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

AK74. GOLOB, Janvit, LIKOZAR, Blaž, KOZLEVČAR, Bojan, FRANCETIČ, Vojmir, NOGRAŠEK, Boštjan, DEVETAK, Marko. *Razvoj tehnologij enkapsulacije gnojil : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 22 f., ilustr. [COBISS.SI-ID 34475269]

PATENTNA PRIJAVA / PATENT APPLICATION

AK75. LUNDER, Mojca, RAVNIKAR, Matjaž, ŠTRUKELJ, Borut, BERLEC, Aleš, ČEH, Boris. *Genetically modified food grade microorganism for treatment of inflammatory bowel disease : Applicant's reference P003127EP*. Munich: European Patent Organisation, 7. January 2010. 8 str. [COBISS.SI-ID 2770801]

AK76. TUREL, Iztok, KLJUN, Jakob, ŠTEFANE, Bogdan. *Postopek za pripravo racemnega nikotina : št. P-201000450*. Ljubljana: Urad Republike Slovenije za intelekturalno lastnino, 22.12.2010. 7 str. [COBISS.SI-ID 34764549]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

AK77. TUREL, Iztok. *Interactions of metal ions with selected biologically active ligands : [Charles University in Prague, Faculty of Mathemathics and Physics, 29. 4. 2010]*. Prague, 2010. [COBISS.SI-ID 33984773]

AK78. PERDIH, Franc. *Organometallic fluorides – overview on synthesis, supramolecular self-assembly and host-guest complexation : [Masaryk University, Department of Chemistry, Brno, Czech Republic, 30. 9. 2010]*. Brno, 2010. [COBISS.SI-ID 34487045]

VABLJENO PREDAVANJE NA KONFERENCI BREZ NATISA / UNPUBLISHED INVITED CONFERENCE LECTURE

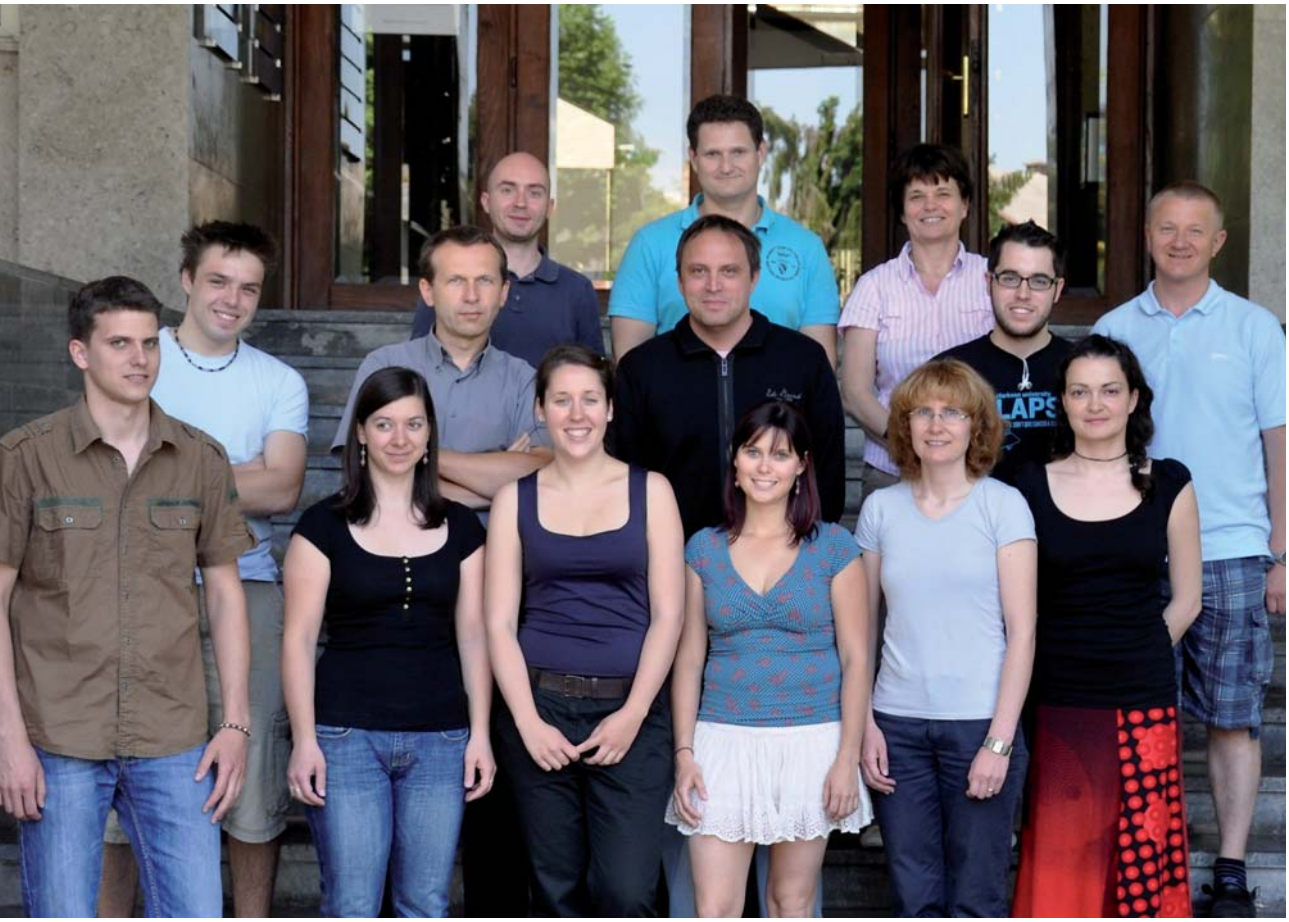
AK79. BUKOVEC, Nataša. *Uporaba titanovega dioksida v vsakdanjem življenju in sodobnih tehnologijah : 2. simpozij učiteljev in laborantov kemije v srednjih šolah, Kope, 2010*. Kope, 2010. [COBISS.SI-ID 34342405]

AK80. TRATAR-PIRC, Elizabeta. Vloga makro in mikro-elementov pri ohranjanju zdravja : 2. simpozij učiteljev in laborantov kemije v srednjih šolah, Kope, 2010. Kope, 2010. [COBISS.SI-ID 34342917]

UREDNIK / EDITORSHIP

AK81. Nineteenth Slovenian-Croatian Crystallographic Meeting, 18–20 June, 2010, Strunjan, Slovenia, LAH, Nina (ur.), LEBAN, Ivan (ur.). *Book of abstracts [and] programme*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010. 67 str., ilustr. [COBISS.SI-ID 23755815]

AK82. *Metal-based drugs*. Turel, Iztok (član uredniškega odbora 2001-2002, član uredniškega sveta 2006–). Tel Aviv: Freund Publishing House. ISSN 0793-0291. [COBISS.SI-ID 759343]



KATEDRA ZA BIOKEMIJO
CHAIR OF BIOCHEMISTRY

PREDSTOJNICA KATEDRE / HEAD

prof. dr. Brigita Lenarčič

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Brigita Lenarčič
doc. dr. Marko Dolinar
doc. dr. Gregor Gunčar

v dopolnilnem razmerju / *part-time*
prof. dr. Tamara Lah Turnšek
prof. dr. Vladka Čurin Šerbec
izr. prof. dr. Kristina Djinović Carugo
prof. dr. Roman Jerala
izr. prof. ddr. Boris Turk
izr. prof. dr. Janez Plavec
prof. dr. Igor Križaj
izr. prof. dr. Metka Renko (upokojena / *retired)*)

Asistenti / Assistants
Marina Klemenčič, univ. dipl. biokem.
dr. Marko Novinec
dr. Nika Lovšin
dr. Miha Pavšič
dr. Petra Prijatelj Žnidaršič
dr. Vera Župunski

Tehnik / Technician
Matjaž Malavašič

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Sara Drmota	K. Djinović Carugo	2010–2014	doktorski študij / *PhD*
Katja Hrovat Arnež	G. Gunčar	2010–2014	doktorski študij / *PhD*
Nataša Lindič	N. Lovšin	2009–2013	doktorski študij / *PhD*
Nives Škrlj	M. Dolinar	2006–2011	doktorski študij / *PhD*
Tilen Vidmar	B. Lenarčič	2010–2014	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemija / *Chemistry* – UN:
Molekularne osnove ved o življenju / *Molecular Fundamentals of Life Sciences*
Biološka kemija / *Biological Chemistry*

Biokemija / Biochemistry – UN:
Temelji biokemije / *Biochemistry Fundamentals*
Biokemijski praktikum / *Biochemistry Practicals*
Biokemija / *Biochemistry*
Molekularna biologija / *Molecular Biology*
Biokemijska informatika / *Bioinformatics*

Kemijsko inženirstvo / *Chemical Engineering* – UN:
Molekularne osnove ved o življenju / *Molecular Fundamentals of Life Sciences*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Encimatika / *Enzymology* – UN
Tehnologija rekombinantne DNA / *Recombinant DNA Technology* – UN
Molekularna imunologija / *Molecular Immunology* – UN
Biokemija / *Biochemistry* – UN
Metode določanja 3D strukture makromolekul / *Methods of Macromolecular 3D Structure Determination* – UN
Encimska tehnologija / *Enzyme Technology* – UN
Biološke membrane / *Biological Membranes* – UN
Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UN
Regulacija metabolizma / *Regulation of Metabolism* – UN
Biokemija raka / *Biochemistry of Cancer* – UN
Encimi / *Enzymes* – UN
Biokemija II / *Biochemistry II* – UN

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Sodobne metode in tehnike v biokemiji / *Modern Methods and Techniques in Biochemistry*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Biokemija / *Biochemistry* FFA – UN – Laboratorijska biomedicina / *Laboratory Biomedicine*

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Izbrani procesi v biokemiji in molekularni biologiji / *Selected Advanced Topics in Biochemistry and Molecular Biology* (UL Interdisciplinarni doktorski študijski program Biomedicina / *UL Interdisciplinary Doctoral Study Programme in Biomedicine)*

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

Raziskovalno delo članov katedre poteka na petih raziskovalnih projektih ter v okviru treh raziskovalnih programov: Toksini in biomembrane, Proteoliza in njena regulacija ter Strukturna biologija. Pri vseh treh večina raziskav poteka na odsekih Instituta »Jožef Stefan«.

Člani katedre, ki se ukvarjajo s toksinologijo, raziskujejo evolucijsko zgodovino, dinamiko in mehanizme delovanja transpozicijskih elementov ter odnose struktura – funkcija pri različnih toksinih.

Sodelavci, ki so vključeni v programa Proteoliza in njena regulacija ter Strukturna biologija, analizirajo proteaze in njihove inhibitorje, tako naravnega izvora kakor tiste, ki jih pridobijo s tehnikami rekombinantne DNA. Poudarek je na študijah interakcij proteaz z novimi inhibitorji ter odnosom med strukturo in funkcijo pri teh interakcijah. V zadnjem času se ukvarjamo tudi z raziskavami mehanizmov alosterične regulacije ter konformacijske fleksibilnosti nekaterih proteaz.

Nadaljujemo s podrobnimi strukturnimi študijami človeške epitelijske celične adhezijske molekule EpCAM, raziskave pa smo z njenega zunajceličnega dela razširili tudi na kratek znotrajcelični del. Z obdelavo že dobljenih strukturnih podatkov načrtujemo nove eksperimente, s katerimi želimo pojasniti mehanizem delovanja te molekule pri celični adheziji in signaliziranju.

Proteini APOBEC3 (A3) preprečujejo razmnoževanje številnim eksogenim in endogenim retrovirusom ter retrotranspozonom. V naši skupini raziskujemo, kako preprečujejo razmnoževanje retrotranspozonom z uporabo celičnih kultur kot tudi s študijami na živalskih modelih. Ugotovili smo, da proteini A3 preprečujejo razmnoževanje retrotranspozonom tik pred njihovo vključitvijo v genom in, da zato encimska aktivnost ni potrebna.

Nadaljevali smo s pripravo humaniziranih oblik rekombinantnih enoverižnih fragmentov protiteles, specifičnih za patogeno obliko prionskega proteina. Delo poteka v sodelovanju z Zavodom za transfuzijsko medicino (skupina prof. dr. Vladke Čurin Šerbec) ter začeli s pripravo modificiranih oblik, ki vključujejo peptidne oznake za prehod krvno-možganske pregrade.

The Chair is engaged in five research projects running within three different research programmes at the Jožef Stefan Institute: Toxins and Biomembranes, Proteolysis and its Regulation, and Structural Biology.

The research on toxinology focuses on the evolution, dynamics and mechanisms of transposition elements and on structure – function investigations of toxin proteins.

Those working on the Proteolysis and Structural Biology programmes are analysing proteases and their inhibitors of natural origin as well as those obtained by recombinant DNA techniques. We focus primarily on identifying and characterizing novel protease inhibitors and on studying the structure-function relationships behind these interactions. Recently, we have also started studying the mechanisms of allosteric regulation and conformational flexibility in some proteases.

We have expanded our research on human epithelial cell adhesion molecule EpCAM, particularly structural studies, to cover also its small intracellular part in addition to the extracellular part. Structural data that has been obtained form a solid basis for new experiments designed to tackle the mechanism underlying EpCAM-mediated cell adhesion and signalling.

APOBEC3 (A3) proteins are potent host restriction factors against various exogenous and endogenous retroviruses including retrotransposons. We extensively study the mechanism of their inhibition in mammalian cell culture system as well as in vivo. Our studies revealed that human A3 proteins inhibit pre-integration independently of their enzymatic activity.

As part of cooperation with the Blood Transfusion Centre of Slovenia we continued with the preparation of humanized forms of recombinant single-chain antibody fragments directed against the pathogenic form of the prion protein. In this context we started preparing modified forms which include peptide tags for passage across the blood-brain barrier.

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

T. Lah Turnšek je prejela Lapanjetovo nagrado Slovenskega biokemijskega društva za vrhunske dosežke na področju biokemijskih znanosti, predvsem za dolgoletne raziskave fiziološke vloge proteinaz, največ v povezavi z rakavimi obolenji.

T. Lah Turnšek was recipient of the Lapanje Prize, awarded by the Slovenian Biochemical Society, for her outstanding achievements in the field of biochemical sciences, especially for her research on the physiological role of proteinases, mostly in connection with cancer.

R. Jerala je bil vodja ekipe študentov, ki so novembra 2010 osvojili prvo mesto na mednarodnem tekmovanju iz sintezne biologije iGEM. Na srečanju ekip, ki je potekalo na univerzi MIT (Cambridge, ZDA) je med 130 prijavljenimi ekipami z vsega sveta osvojila najvišje priznanje, hkrati pa je bila najboljša v kategoriji Nove aplikacije, prispevala pa je tudi najboljši načrtovani genetski element (BioKocko). Članica študentske raziskovalne ekipe je bila tudi študentka Biokemije Tina Ilc.

R. Jerala was the supervisor of the student team which won the Grand Prize at the International synthetic biology iGEM competition in November 2010. At the jamboree organized by the MIT (Cambridge, USA) our team received the top award among 130 competing teams from around the globe. In addition, the team was the best in the category New Applications and it contributed the best new BioBrick part/device. A member of the student research team was Tina Ilc, our student of biochemistry.

I. Križaj je bil mentor Lidije Kovačič, ki je prejela Nagrado Maksa Samca za doktorsko disertacijo s področja biokemije. To nagrado podeljuje Fakulteta za kemijo in kemijsko tehnologijo za izjemno uspešno raziskovalno delo v obdobju priprave doktorata.

I. Križaj was the mentor of Lidija Kovačič, who won the Maks Samec Award for doctoral thesis in the field of biochemistry. This prize is awarded by the Faculty of Chemistry and Chemical Technology for outstanding research in preparing the PhD thesis.

V. Čurin Šerbec je bila somentorica Katje Trontelj, ki je prejela Krkino nagrado za doktorsko delo (mentor D. Miklavčič).

V. Čurin Šerbec was co-mentor of Katja Trontelj who was the recipient of the Krka Award for her PhD thesis (mentor D. Miklavčič).

Univerzitetno Prešernovo nagrado za leto 2010 je dobila Saša Jereb, študentka biokemije, za raziskovalno delo s področja sintezne biokemije. Delo z naslovom »Razvoj od mutacij neodvisnega zaznavanja virusa HIV« je pripravila pod mentorstvom R. Jerale.

Saša Jereb, a Biochemistry student, received the University Prešeren Award in 2010 for her research in synthetic biology ("Development of mutation-independent detection of HIV virus") under the mentorship of R. Jerala.

Prešernovo nagrado FKKT za leto 2010 so prejeli / *The Faculty Prešeren Award recipients for 2010 were*:

- Katja Goričar (mentorica A. Plemenitaš, somentorica V. Dolžan)
- Marija Kokalj (mentorica V. Čurin Šerbec)
- Anja Lukan (mentor M. Dolinar, somentorica K. Drobnič)

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Hlajeni centrifugi Haereus in Eppendorf /*Refrigerated Centrifuges Haereus and Eppendorf*
- Hlajena mikrocentrifuga Eppendorf / *Refrigerated Microcentrifuge Eppendorf*
- Dva spektrofotometra UV/VIS Pharmacia Ultrospec 1000 z računalniško podporo / *Two Spectrophotometers UV / VIS Pharmacia Ultrospec 1000 with Computer Support*
- Spektrofotometer UV/VIS Cary 50 z računalniško podporo / *Spectrophotometer UV/VIS Cary 50 with Computer Support*
- Fluorimeter Perkin-Elmer LS 50 z računalniško podporo / *Fluorimeter Perkin-Elmer LS 50 with Computer Support*
- Fluorimeter Aminco / *Fluorimeter Aminco*
- Aparatura »stopped flow« za določanje encimske kinetike / *Stopped-Flow Enzyme Kinetics Apparatus*
- Inkubator za kristalizacijske plošče Molecular Dimensions / *Incubator for Crystallization Trays Molecular Dimensions*
- Kristalizacijski robot Crystal Gryphon (96-kanalni) / *Crystallization Robot (96 Channels) Crystal Gryphon*
- Čitalnik mikrotitrskih ploščic Tecan Sunrise / *Microtiter Plate Reader Tecan Sunrise*
- Aparaturi za PCR Applied Biosystems GeneAmp 2700 in Veriti / *PCR Apparatures Applied Biosystems GeneAmp 2700 and Veriti*

- Spektrofotometer za majhne volumne vzorcev (NanoDrop) / *Spectrophotometer for Small Sample Volumes (NanoDrop)*
- Ultrazvočni homogenizer / *Ultrasound Homogenizer*
- Elektroporator / *Electroporator*
- Naprave za elektroforezno analizo proteinov in prenos Western / *Instruments for Electrophoretic Separations of Proteins and Western Blotting*
- Elektroforezni sistem Phast */ Phast Electrophoresis System*
- Naprave za agarozno gelsko elektroforezo DNA / *Instruments for DNA Agarose Gel Electrophoresis*
- Transiluminator / *Transilluminator*
- Sistem za dokumentacijo elektroforeznih gelov / *Electrophoresis Documentation System*
- Suhi inkubator in stresalnik za mikrobiologijo / *Incubator/Shaker*
- Hlajeni inkubator s stresalnikom / *Cooled Incubator/Shaker*
- CO_2 inkubator / *CO_2 Incubator*
- Stereo mikroskop M7.5 Leica / *Stereo Microscope M7.5 Leica*
- Invertni mikroskop CKX-41 Olympus / *Inverted Microscope CKX-41 Olympus*
- Mešalniki in vibracijski stresalniki / *Mixers and Shakers*
- Analitske tehtnice / *Analytical Balances*
- Čiste komore / *Clean Chambers*
- pH meter Mettler-Toledo */ pH Meter Mettler-Toledo*
- Tekočinska kromatografija za hitro ločevanje proteinov FPLC / *Fast Protein Liquid Chromatograpy (FPLC) GE Healthcare*
- Tekočinska kromatografija za hitro ločevanje proteinov Acta Prime / *Acta Prime Protein Liquid Chromatography System*
- Tekočinska kromatografija visoke ločljivosti (HPLC) / *High Performance Liquid Chromatography (HPLC)*
- Frakcijski kolektor / *Fraction Collector*
- Vakuumski koncentrator / *Vac Concentrator*
- Ledomat za drobljeni led */ Flaked Ice Machine*
- Termostatirana vodna kopel */ Thermostated Water Bath*
- Avtoklav / *Autoclave*
- Zmrzovalnik –80 °C / *Freezer –80 °C*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P1–0207	Toksini in biomembrane / *Toxins and Biomembranes* Vodja programa / *Principal Researcher*: I. Križaj (IJS)
P1–0140	Proteoliza in njena regulacija / *Proteolysis and its Regulation* Vodja programa / *Principal Researcher*: B. Turk (IJS)

P1–0048 Strukturna biologija / *Structural Biology*
Vodja programa / *Principal Researcher*: D. Turk (IJS)

TEMELJNI PROJEKTI / BASIC RESARCH

J1–2017 Epitelijska celična adhezijska molekula (EpCAM) – tarča tumorske terapije: struktura, proteolitično procesiranje in interakcija z drugimi proteini / *Epithelial Cell Adhesion Molecule (EpCAM), a Target for Tumor Therapy: Structure, Proteolytic Processing and Interaction with Other Proteins*
Nosilka / *Principal Researcher*: B. Lenarčič

J7–2230 Protivirusni proteini APOBEC3 in njihova vloga pri obrambi proti retroelementom / *APOBEC3 Antiviral Proteins and Their Role in the Defence Against Retroelements*
Nosilka / *Principal Researcher*: N. Lovšin

J1–2141 Regulatorna genomika: nastanek in evolucija kompleksnega transkripcijskega regulatornega omrežja pri vretenčarjih / *Regulatory Genomics: Emergence and Evolution of a Complex Regulatory Network in Vertebrates*
Nosilec / *Principal Researcher*: D. Kordiš

J1–0841 Antikancerogeno delovanje bioaktivnih spojin cianobakterijskega izvora v napredovanju možganskih tumorjev –gliobastomov / *Anticarcinogenic Activity of Bioactive Compounds from Cyanobacterial Source in the Progression of Brain Tumours – Glioblastoma*
Nosilka / *Principal Researcher*: T. Lah Turnšek

APLIKATIVNI PROJEKTI / APPLIED RESARCH

L3–0206 Prioni v humani medicini: od strukturnih študij do aplikacij / *Prions in Human Medicine: From Structural Studies to Applications*
Nosilka / *Principal Researcher*: V. Čurin Šerbec
Sofinancer / *Co-sponsored by*: DiaMed, Benelux

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

BIO1. KHAN, Muhammad Bashir, SJOBLOM, Bjoern, SCHWEYEN, Rudolf J., DJINOVIĆ CARUGO, Kristina. Crystallization and preliminary X-ray diffraction analysis of the N-terminal domain of Mrs2, a magnesium ion transporter from yeast inner mitochondrial membrane. *Acta crystallographica. Section F, Structural biology and crystallization communications*, 2010, vol. 66, part 6, str. 658–661. [COBISS.SI-ID 516142361]

BIO2. SVIDOVÁ, Soňa, SPONDER, Gerhard, SCHWEYEN, Rudolf J., DJINOVIĆ CARUGO, Kristina. Functional analysis of the conserved hydrophobic gate region of the magnesium transporter CorA. *Biochim. biophys. acta, Biomembr.*. [Print ed.], str. 1–5. doi: 10.1016/j.bbamem.2010.10.017. [COBISS.SI-ID 34712837]

BIO3. KOSTAN, Julius, SJÖBLOM, Björn, MAIXNER, Frank, MLYNEK, Georg, FURTMÜLLER, Paul Georg, OBINGER, Christian, WAGNER, Michael, DAIMS, Holger, DJINOVIĆ CARUGO, Kristina. Structural and functional characterisation of the chlorite dismutase from the nitrite-oxidizing bacterium »Candidatus Nitrospira defluvii« : identification of a catalytically important amino acid residue. *J Struct Biol*, 2010, vol. 172, no. 3, str. 331–342. [COBISS.SI-ID 34713349]

BIO4. DJINOVIĆ CARUGO, Kristina, CARUGO, Olivero. Structural portrait of filamin interaction mechanisms. *Current protein and peptide science*, 2010, vol. 11, no. 7, str. 639–650. [COBISS.SI-ID 34715141]

BIO5. CHEN, Wei-Qiang, SALMAZO, A., MYLLYKOSKI, Matti, SJÖBLOM, Björn, BIDLINGMAIER, Martin, POLLAK, Arnold, BAUMGÄRTEL, Peter, DJINOVIĆ CARUGO, Kristina, KURSULA, Petri, LUBEC, Gert. Purification of recombinant growth hormone by clear native gels for conformational analyses : preservation of conformation and receptor binding. *Amino acids*, 2010, vol. 39, no. 3, str. 859–869. [COBISS.SI-ID 34717957]

BIO6. ŠKRLJ, Nives, VIDRIH, Zlatko, DOLINAR, Marko. A universal approach for promoter strength evaluation supported by the web-based tool PromCal. *Anal. biochem.*, 2010, vol. 396, no. 1, str. 83–90. [COBISS.SI-ID 33430789]

BIO7. ŠKRLJ, Nives, ČURIN-ŠERBEC, Vladka, DOLINAR, Marko. Single-chain Fv antibody fragments retain binding properties of the monoclonal antibody raised against peptide P1 of the human prion protein. *Appl. biochem. biotechnol.*, 2010, issue 6, vol. 160, str. 1808–1821. [COBISS.SI-ID 30601477]

BIO8. NOVINEC, Marko, KOVAČIČ, Lidija, LENARČIČ, Brigita, BAICI, Antonio. Conformational flexibility and allosteric regulation of cathepsin K. *Biochem. j. (Lond., 1984)*, 2010, vol. 429, no. 2, str. 379–389. [COBISS.SI-ID 34035973]

BIO9. POŽGAN, Urška, CAGLIČ, Dejan, ROZMAN, Blaž, NAGASE, Hideaki, TURK, Vito, TURK, Boris. Expression and activity profiling of selected cysteine cathepsins and matrix metalloproteinases in synovial fluids from patients with rheumatoid arthritis and osteoarthritis. *Biol Chem*, 2010, vol. 391, no. 5, str. 571–579. [COBISS.SI-ID 23546151]

BIO10. PUCER, Anja, CASTINO, Roberta, MIRKOVIĆ, Bojana, FALNOGA, Ingrid, ŠLEJKOVEC, Zdenka, ISIDORO, Ciro, LAH TURNŠEK, Tamara. Differential role of cathepsins B and L in autophagy-associated cell death induced by arsenic trioxide in U87 human glioblastoma cells. *Biol Chem*, 2010, vol. 391, 13 str., [in press]. [COBISS.SI-ID 2213967]

BIO11. NISHIMURA, Agnes L., ŽUPUNSKI, Vera, ROGELJ, Boris. Nuclear import impairment causes cytoplasmic trans-activation response DNA-binding protein accumulation and is associated with frontotemporal lobar degeneration. *Brain*, 2010, issue 6, vol. 133, str. 1763–1771. [COBISS.SI-ID 23645223]

BIO12. KASTELIC, Jože, HODNIK, Žiga, ŠKET, Primož, PLAVEC, Janez, LAH, Nina, LEBAN, Ivan, PAJK, Matjaž, PLANINŠEK, Odon, KIKELJ, Danijel. Fluconazole cocrystals with dicarboxylic acids. *Cryst. growth des.*, 2010, vol. 10, no. 11, str. 4943–4953. [COBISS.SI-ID 2881905]

BIO13. GAŠPERŠIČ, Jernej, HAFNER BRATKOVIČ, Iva, STEPHAN, Michel, VERANIČ, Peter, BENČINA, Mojca, VORBERG, Ina, JERALA, Roman. Tetracysteine-tagged prion protein allows discrimination between the native and converted forms. *FEBS journal*, 2010, vol. 277, no. 9, str. 2038–2050. [COBISS.SI-ID 4377626]

BIO14. RABELO MELO, Fabio, TURK, Boris, PEJLER, Gunnar. A role for serglycin proteoglycan in mast cell apoptosis induced by a secretory granule-mediated pathway. *J Biol Chem*, [in press] 2010, 13 str. [COBISS.SI-ID 24226855]

BIO15. MOHORČIČ, Martina, JERMAN, Ivan, ZORKO, Mateja, BUTINAR, Lorena, OREL, Boris, JERALA, Roman, FRIEDRICH, Jožica. Surface with antimicrobial activity obtained through silane coating with covalently bound polymyxin B. *J. mater. sci., Mater. med.*, 2010, vol. 21, issue 10, str. 2775–2782. [COBISS.SI-ID 4471578]

BIO16. LAH TURNŠEK, Tamara, NANNI, Isabelle, TRINKAUS, Miha, METELLUS, Philipe, DUSSERT, Christophe, RIDDER, Leo de, RAJČEVIĆ, Uroš, BLEJEC, Andrej, MARTIN, Pierre-Marie. Toward understanding recurrent meningioma: the potential role of lysosomal cysteine proteases and their inhibitors. *J. neurosurg.*, 2010, vol. 112, no. 5, str. 940–950. [COBISS.SI-ID 2079567]

BIO17. ŠKET, Primož, PLAVEC, Janez. Tetramolecular DNA quadruplexes in solution : insights into structural diversity and cation movement. *J. Am. Chem. Soc.*, 2010, vol. 132, no. 36, str. 12724–12732.[COBISS.SI-ID 4487962]

BIO18. GALKIN, Vitold E., ORLOVA, Albina, SALMAZO, Anita, DJINOVIĆ CARUGO, Kristina, EGELMAN, Edward H. Opening of tandem calponin homology domains regulates their affinity for F-actin. *Nature structural & molecular biology*. Online ed., 2010, vol. 17, issue 5, str. 614–616. [COBISS.SI-ID 516155161]

BIO19. PODBEVŠEK, Peter, ALLERSON, Charles R., BHAT, Balkrishen, PLAVEC, Janez. Solution-state structure of a fully alternately 2'-F/2'-OMe modified 42-nt dimeric siRNA construct. *Nucleic acids res.*, 2010, vol. 38, no. 20, str. 7298–7307. [COBISS.SI-ID 4541466]

BIO20. ILC, Gregor, GIACHIN, Gabriele, JAREMKO, Mariusz, JAREMKO, Łukasz, BENETTI, Federico, PLAVEC, Janez, ZHUKOV, Igor, LEGNAME, Giuseppe. NMR Structure of the Human Prion Protein with the Pathological Q212P Mutation Reveals Unique Structural Features. *PLoS one*, jul. 2010, vol. 5, no. 7, str. e11715-1-e11715-15, ilustr. [COBISS.SI-ID 4449050]

BIO21. CEVEC, Mirko, THIBAUDEAU, Christophe, PLAVEC, Janez. NMR structure of the let-7 miRNA interacting with the site LCS1 of lin-41 mRNA from Caenorhabditis elegans. *Nucleic acids res.*, 2010, vol. 38, no. 21, str. 7814–7821, ilustr. [COBISS.SI-ID 4554778]

BIO22. MAKUC, Damjan, ALBRECHT, Markus, PLAVEC, Janez. Conformational changes of functionalised indole receptors upon their interaction with anions. *Supramol. chem. (Print)*, 2010, vol. 22, no. 10, str. 603–611. [COBISS.SI-ID 4528922]

BIO23. SAUL, Friderick A., PRIJATELJ, Petra, NORMAND, Brigitte V. de, VILLETTE, Benoit, RAYNAL, Bertrand, PUNGERČAR, Jože, KRIŽAJ, Igor, FAURE, Grazyna. Comparative structural studies of two natural isoforms of Ammodytoxin, phospholipases A_2 from *Vipera ammodytes ammodytes* which differ in neurotoxicity and anticoagulant activity. *J Struct Biol*, 2010, vol. 169, no. 3, str. 360–369. [COBISS.SI-ID 23047975]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

BIO24. TURK, Boris. *Cysteine cathepsins : friends and foes : invited talk.* Wroclaw: University of Wroclaw, 19. okt. 2010. [COBISS.SI-ID 24132647]

BIO25. KRIŽAJ, Igor. *Fosfolipaze A2 iz modrasovega strupa : od strukturne karakterizacije do uporabe pri analizi patofiziologije sesalnih ortologov : vabljeno predavanje*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 10. nov. 2010. [COBISS.SI-ID 24176423]

BIO26. TURK, Boris. *Protease signals – a point for therapeutic intervention : invited talk.* Gent: University of Gent, 20. maj 2010. [COBISS.SI-ID 23702311]

VABLJENO PREDAVANJE NA KONFERENCI BREZ NATISA / UNPUBLISHED INVITED CONFERENCE LECTURE

BIO27. TURK, Boris. *Nanodelci in njihova uporabnost : varnost pri delu z nanodelci, vpliv na zdravje in uporabnost nanodelcev v medicini : 6. nanotehnološki dan, 17. september 2010, Ljubljana, Slovenija*. 2010. [COBISS.SI-ID 23986215]

BIO28. TURK, Boris. *Razumevanje življenskih procesov s pomočjo biokemijskega znanja : 16. festival znanosti, 21.–23. avgust, 2010, Ljubljana*. 2010. [COBISS.SI-ID 23986471]

BIO29. KRIŽAJ, Igor. *Secretory phospholipases A2 in health and disease : presented at CIPKeBiP Startup Conference, 15–16 March, 2010, Ljubljana, Slovenia*. 2010. [COBISS.SI-ID 23484967]

BIO30. LAH TURNŠEK, Tamara. *Pomen matičnih celic pri raku : [predavanje na prireditvi Raziskovalni dan Fakultete za farmacijo, 1.12.2010]*. 2010. [COBISS.SI-ID 2314575]

UREDNIK / EDITORSHIP

BIO31. 6th Conference on Experimental and Translational Oncology, Kranjska gora, Slovenia, March, 24–28, 2010, SERŠA, Gregor (ur.), KOS, Janko (ur.), LAH TURNŠEK, Tamara (ur.), KRANJC, Simona (ur.). *Book of abstracts*. Ljubljana: Association of Radiology and Oncology, 2010. 175 str. ISBN 978-961-91302-3-0. [COBISS.SI-ID 250253824]

BIO32. XIIth Symposium on Proteases, Inhibitors and Biological Control, Portorož, Slovenia, September 25–29, 2010, DOLINAR, Marko (ur.), STOKA, Veronika (ur.), TURK, Boris (ur.). *Book of abstracts*. Ljubljana: Jožef Stefan Institute, 2010. 130 str. ISBN 978-961-264-022-4. [COBISS.SI-ID 252579328]

BIO33. VODIŠKAR, Mateja (ur.), PLAVEC, Janez (ur.). *Program and book of abstracts*. Ljubljana: Slovenian NMR Centre, National Institute of Chemistry, 2010. 82 str., ilustr. ISBN 978-961-6104-16-6. [COBISS.SI-ID 251065088]

BIO34. *Biological chemistry*. Turk, Boris (urednik 2008–). Berlin; New York: Walter de Gruyter. ISSN 1431-6730. [COBISS.SI-ID 1541908]

BIO35. *Current pharmaceutical design*. Turk, Boris (gostujoči urednik 2007–). Schiphol: Bentham Science Publishers. ISSN 1381-6128. [COBISS.SI-ID 16094247]

BIO36. *Global toxin review*. Križaj, Igor (član uredniškega odbora 2005–). [S. l.]: globaltoxin.org, 2005–. [COBISS.SI-ID 21976615]

BIO37. *Journal of biological engineering*. Dolinar, Marko (član uredniškega odbora 2008–). London: BioMed Central. ISSN 1754-1611. [COBISS.SI-ID 30190597]

BIO38. *Journal of venom research*. Križaj, Igor (član uredniškega odbora 2010–). Oxford: 2010–. [COBISS.SI-ID 23582247]

BIO39. *The open toxinology journal*. Križaj, Igor (član uredniškega odbora 2008–). Saif Zone, Sharjah, U.A.E.: Bentham Open, 2008–. [COBISS.SI-ID 21915431]

BIO40. *Poročilo o delu – Nacionalni inštitut za biologijo*. Lah, Tamara (član uredniškega odbora 1995–). Ljubljana: Inštitut za biologijo, 199?–. ISSN 1408-3299. [COBISS.SI-ID 68115968]

BIO41. *Radiology and oncology*. Lah Turnšek, Tamara (član uredniškega odbora 2007–). Ljubljana: Slovenian Medical Society – Section of Radiology; [Zagreb]: Croatian Medical Association – Croatian Society of Radiology, 1992–. ISSN 1318-2099. [COBISS.SI-ID 32649472]

BIO42. *Toxicon*. Križaj, Igor (član uredniškega odbora 2006–). [Print ed.]. Oxford: Pergamon press, 1962–. ISSN 0041-0101. [COBISS.SI-ID 1835012]

KATEDRA ZA FIZIKALNO KEMIJO
CHAIR OF PHYSICAL CHEMISTRY

PREDSTOJNICA KATEDRE / HEAD

izr. prof. dr. Ksenija Kogej

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Marija Bešter Rogač
izr. prof. dr. Andrej Jamnik
izr. prof. dr. Ksenija Kogej
prof. dr. Jože Koller
izr. prof. dr. Jurij Lah
prof. dr. Ciril Pohar
prof. dr. Jože Škerjanc, zaslužni profesor (upokojen) / *Professor Emeritus*
prof. dr. Gorazd Vesnaver
prof. dr. Vojeslav Vlachy

Asistenti / Assistants
dr. Matjaž Bončina
doc. dr. Janez Cerar
dr. Andrej Godec
izr. prof. dr. Barbara Hribar Lee
dr. Miha Lukšič
dr. Črtomir Podlipnik
dr. Iztok Prislan
doc. dr. Jurij Reščič
Bojan Šarac, univ. dipl. kem.
doc. dr. Matija Tomšič
doc. dr. Tomaž Urbič

Raziskovalka / Researcher
dr. Jožica Dolenc

Tehniki / Technicians
Anton Kelbl
Anton Kokalj
Cirila Peklaj

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Alan Bizjak	V. Vlachy	2005–2010	doktorski študij / *PhD*
Igor Drobnak	A. Jamnik	2006–2011	doktorski študij / *PhD*
Andrej Lajovic	V. Vlachy	2007–2012	doktorski študij / *PhD*
Sašo Čebašek	V. Vlachy	2009–2013	doktorski študij / *PhD*
Simona Prelesnik	K. Kogej	2009–2013	doktorski študij / *PhD*
Ana Kroflič	M. Bešter Rogač	2009–2013	doktorski študij / PhD
Andrej Mernik	J. Lah	2010–2014	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemija / *Chemistry* – UN:
Fizikalna kemija I, II / *Physical Chemistry I, II*
Praktikum iz fizikalne kemije / *Practicum in Physical Chemistry*
Struktura atomov in molekul / *Structure of Atoms and Molecules*

Biokemija / *Biochemistry* – UN:
Fizikalna kemija I, II / *Physical Chemistry I, II*
Struktura atomov in molekul / *Structure of Atoms and Molecules*

Kemijsko inženirstvo / *Chemical Engineering* – UN:
Kemijska termodinamika / *Chemical Thermodynamics*

Tehniška varnost / *Technical Safety* – UN:
Numerične metode v varnosti I / *Numerical Methods in Technical Safety I*

Kemijska tehnologija / *Chemical Technology* – VS:

Praktikum iz kemije / *General Chemistry – Practical Course*

Fizikalna kemija I / *Physical Chemistry I*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Fizikalna kemija / *Physical Chemistry* – UN in VS

Fizikalna kemija II / *Physical Chemistry II* – UN

Delovno okolje – prah (aerosoli) / *Working Environment – Aerosols* – VS

Praktikum – uvod v prakso / *Introduction to Practical Work* – VS

Merjenje in regulacija / *Measurements* and *Regulations* – VS

Fizikalna kemija in meritve / *Physical Chemistry and Measurements* – VS

Površinska in koloidna kemija / *Surface and Colloid Chemistry* – UN

Struktura atomov in molekul / *Structure of Atoms and Molecules* – UN

Instrumentalne metode / *Instrumental Methods* – UN

Makromolekulska kemija / *Macromolecular Chemistry* – UN

Merjenje, regulacija, avtomatizacija / *Measurement, Regulations, Automation* – UN

Biofizikalna kemija / *Biophysical Chemistry* – UN

Metodika eksperimentov v fizikalni kemiji / *Methodology of Experiments in Physical Chemistry* – UN

Bolonjski programi 2. stopnje / *Bologna 2nd Cycle Master Study Programmes*

Tehniška varnost / *Technical Safety*:

Numerične metode v varnosti II / *Numerical Methods in Technical Safety II*

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Izbrana poglavja iz eksperimentalne fizikalne kemije / *Selected Topics in Experimental Physical Chemistry*

Teoretične metode v fizikalni kemiji / *Theoretical Methods in Physical Chemistry*

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Raztopine elektrolitov / *Solution Electrochemistry*

Sintetski polielektroliti in biopolimeri / *Synthetic Polyelectrolytes and Biopolymers*

Osnove molekulskega modeliranja / *Fundamentals of Molecular Modelling*

Termodinamika raztopin / *Thermodynamics of Solutions*

Fizikalna kemija raztopin makromolekul in koloidov / *Physical Chemistry of Macromolecular and Colloidal Solutions*

Biološke makromolekule / *Biological Macromolecules*

Fizikalna kemija polimerov / *Physical Chemistry of Polymers*

Avtomatska regulacija procesov / *Chemical Process Control*

Biofizikalna kemija / *Biophysical Chemistry*

Statistična termodinamika tekočin in raztopin / *Statistical Thermodynamics of Liquids and Solutions*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Fizikalna kemija FFA – Farmacija UN in Laboratorijska biomedicina UN / *Physical Chemistry – Uniform Master Study Programme in Pharmacy and Undergraduate Study Programme in Laboratory Biomedicine*

Tehnološko procesništvo / *Food Processing Technology* BF – UN

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Fizikalna kemija / *Physical Chemistry* NTF – UN

Fizikalna kemija / *Physical Chemistry* PEF – UN

Fizikalna kemija II / *Physical Chemistry II* PEF – UN

Vaje iz fizikalne kemije / *Physical Chemistry Laboratory* FMF – UN

Bolonjski programi 2. stopnje / *Bologna 2nd Cycle Master Study Programmes*

Fizikalna kemija / *Physical Chemistry* NTF

Fizikalna kemija polimerov / *Physical Chemistry of Polymers* NTF

Fizikalna kemija / *Physical Chemistry* BF

Bolonjski programi 3. stopnje/ *Bologna 3rd Cycle Doctoral Study Programmes*

Koloidna kemija / *Colloid Chemistry* – UL Interdisciplinarni doktorski študijski program Bioznanosti / *UL Interdisciplinary Doctoral Study Programme in Biosciences*

Nanotehnologije in nanobiologija / *Nanotechnology and Nanobiology* – UL Interdisciplinarni doktorski študijski program Bioznanosti / *UL Interdisciplinary Doctoral Study Programme in Biosciences*

Biomolekularna termodinamika / *Biomolecular Thermodynamics* – UL Interdisciplinarni doktorski študijski program Biomedicina / *UL Interdisciplinary Doctoral Study Programme in Biomedicine*

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

1. Raziskave elektrolitov in polielektrolitov / *Research of Electrolytes and Polyelectrolytes*
   - Transportne in strukturne lastnosti vodnih raztopin fulerenskih elektrolitov / *Transport and Structural Properties of Aqueous Solutions of Fullerene Electrolytes*
   - Interakcije med večvalentnimi ioni in topilom / *Interactions of Multivalent Ions with Solvent*
   - Termodinamične in transportne lastnosti različnih stereoregularnih polielektrolitov / *Thermodynamic and Transport Properties of Different Stereoregular Polyelectrolytes*
   - Termodinamične in transportne lastnosti raztopin ionenov z različnimi protiioni / *Transport Properties of Ionene Solutions with Different Counter Ions*
   - Raziskave soli polianetolesulfonske kisline / *Studies of Polyanetholesulfonic Acid and its Alkaline Salts*
   - Interakcije med površinsko aktivnimi snovmi in polielektroliti / *Interactions Among Surface Active Compounds and Polyelectrolytes*
   - Termodinamske raziskave asociacijskih procesov v raztopinah elektrolitov / *Thermodynamic Investigations of Association in Electrolyte Solutions*

2. Lastnosti raztopin biološko pomembnih molekul / *Properties of Solutions of Biologically Important Molecules*
   - Termodinamika molekulskega prepoznavanja biološko pomembnih molekul / *Thermodynamics of Molecular Recognition of Biologically Important Molecules*
   - Termodinamska stabilnost in interakcije biološko pomembnih molekul v povezavi z njihovimi strukturnimi značilnostmi / *Thermodynamic Stability and Interaction of Biologically Important Molecules and Correlation with their Structural Properties*
   - Termodinamične in strukturne lastnosti raztopin proteinov HSA in lizocima / *Thermodynamic and Structural Properties of Protein Solutions*
3. Raziskave strukturnih in dinamičnih lastnosti koloidnih sistemov in kompleksnih fluidov / *Structure and Dynamics of Colloidal Systems and Complex Fluids*
4. Teoretične raziskave vodnih raztopin / *Theoretical Research of Aqueous Solutions*
   - Adsorpcija vodnih raztopin elektrolitov v neurejeni snovi; Dinamika in struktura / *Electrolyte Adsorption in a Disordered Material; Dynamics and Structure*
   - Lastnosti vode v zaprtih in nehomogenih sistemih / *Properties of Water in Confined and Inhomogeneous Systems*
   - Modeli vode in raziskave hidratacije preprostih topljencev / *Modelling Water and Solvation of Simple Solutes*
   - Dvodelčne porazdelitvene funkcije ionov v okolici valjastega poliiona / *Ion Correlations in the Inhomogeneous Atmosphere Surrounding Cylindrical Polyions*
   - Vpliv dielektrične nezveznosti na lastnosti vodnih raztopin micelov / *Potential of Mean Force Between Charged Colloids: Effect of Dielectric Discontinuities*
   - Mešanice modelnih tekočin z adhezivnim privlačnim medmolekulskim potencialom / *Mixtures of Model Liquids. Molecules with Adhesive Intermolecular Potential*
5. Vpliv temperature in dodane soli na termodinamiko micelizacije površinsko aktivnih snovi / *Thermodynamic Study of Salt and Temperature Induced Micelle Formation of Surfactants*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- A. Jamnik, Zoisovo priznanje za pomembne znanstvene dosežke na področju fizikalne kemije / *Zois Recognition for Significant Scientific Achievements in the Field of Physical Chemistry*
- A. Godec, Nagrada Maksa Samca za popularizacijo študijev na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani za leto 2010 / *Maks Samec Award for the Popularization of Studies at the UL FKKT for 2010*
- A. Mernik, Prešernova nagrada FKKT za leto 2010 (mentor J. Lah) / *The Faculty Prešeren Award for 2010*
- J. Koller, pohvala Študentskega sveta za pedagoško delo na smeri Kemija / *Students Award for the Quality of Teaching in Chemistry Study Programme*

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

– M. Bešter Rogač, članica uredniškega odbora / *Editorial Board Member, J. Mol. Liq.* 2008– Amsterdam, Elsevier
– M. Bešter Rogač, področna urednica / *Associate Editor, Acta Chimica Slovenica,* 2003–
– G. Vesnaver, član uredniškega odbora / *Editorial Board Member, Acta Chimica Slovenica*, 1998–

ORGANIZACIJA (ALI SODELOVANJE PRI ORGANIZACIJI) MEDNARODNIH ZNANSTVENIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

– V. Vlachy, član znanstvenega odbora konference z naslovom *»Frontiers of Water Biophysics«* / *Member of the Scientific Committee of the Conference »Frontiers of Water Biophysics«* (May 2010), Trieste, Italy

DRUGO / OTHER

– J. Dolenc, podoktorska štipendija na Zvezni tehniški visoki šoli (ETH), Zürich / *Post Doctoral Fellowship at the ETH, Zürich*

– V. Vlachy, predstavnik Slovenije v EuCheMS (Evropska zveza za kemijske in molekularne vede) za področje fizikalne kemije / *National Representative at the EuCheMS Physical Chemistry Division*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

– Diferenčni dinamični kalorimeter N-DSC II (CSC, ZDA) / *Nano II Differential Scanning Calorimeter II (CSC, USA)*
– UV-VIS Spektrophotometer Cary BIO 100 (Varian, Australia)
– CD Spectrometer 62A DS (Aviv, ZDA)
– Titracijski mikrokalorimeter VP-ITC (Microcal, ZDA) / *Isothermal Titration Microcalorimeter VP-ITC (Microcal, USA)*
– Računalniška gruča iz 13 štirijedrnih 64 bitnih Intel Q9550 procesorjev / *Thirteen- Node Computer Cluster Based on Quad-Core Intel Q9550 CPUs*
– Sistem za merjenje ozkokotnega rentgenskega sipanja / *Small Angle X-Ray Scattering Instrument*
– Fluorimeter: Luminescence Spectrometer LS 50, Perkin Elmer / *Fluorimeter: Luminescence Spectrometer LS 50, Perkin Elmer*
– Membranski osmometer Knauer / *Membrane Osmometer*; *Knauer*
– Osmometer na parni tlak: K-7000, Knauer / *Vapour Pressure Osmometer, K-7000 Knauer*
– Sistem za merjenje gostot tekočin DMA 5000, Paar z nihajočo kapilaro prostornine 1 ml / *Vibrating Tube Densimeter, DMA 5000 Paar (1 ml Cell)*

- Titracijski kalorimeter: 2277 Thermal Activity Monitor, ThermoMetric/ *Titration Calorimeter: 227 Thermal Activity Monitor*
- *LKB 10700 (Flow, Batch) Calorimeter*
- Sistem za precizno merjenje električne prevodnosti raztopin (predtermostat Lauda WK 1400, termostat Lauda UB 40 (+/– 0,003 C), LCR Agilent 4284A, DMM Agilent 3458A z uporovnim termometrom Pt100, set različnih celic) / *System for High-Performance Electrical Conductivity Measurements of Solutions (Circular Cooler LAUDA WK 1400, Thermostat LAUDA UB40 (+/– 0.003C), LCR Agilent 4284A, DM Agilent 4284A, DM Agilent 3458A Attached to Pt100, Set of Conductivity Cells*
- Sistem za merjenje dinamičnega in statičnega sipanja laserske svetlobe 3D DLS, LS Instruments / *3D DLS Spectrometer, LS Instruments*
- Diferenčni difraktometer DnDc 2010, Brookhaven Instruments / *Differential Diffractometer DnDc 2010, Brookhaven Instruments*
- Gostotomer Paar, DMA 5000 / *Paar Densimeter, DMA 5000*
- TV100K termostatirana dvojna enota za gelsko elektroforezo ter Syngen G:BOX temnica s kamero /*TV100K Cooled Twin-Plate Mini-Gel Electrophoresis Unit & Syngen G:BOX Darkroom with a Camera*
- Fluorimeter: Fluorescence Spectrometer LS 55, Perkin Elmer / *Fluorimeter*: *Fluorescence Spectrometer LS 55, Perkin Elmer*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P1–0201 Fizikalna kemija / *Physical Chemistry*
Vodja programa / *Principal Researcher:* V. Vlachy

TEMELJNI PROJEKTI / BASIC RESEARCH

Z1–9576 Simulacije molekulske dinamike nukleinskih kislin: struktura, dinamika in termodinamska stabilnost / *Molecular Dynamics Simulations of Nucleic Acids: Structure, Dynamics and Thermodynamic Stability*
Nosilka / *Principal Researcher*: J. Dolenc

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

BIO 02/2010 Postavljanje platforme za fizikalno-kemijsko karakterizacijo proteinskih učinkovin / *Setting up the Platform for Physico-Chemical Characterization of Protein Substances*
Nosilec / *Principal Researcher*: J. Lah
Financer / *Sponsored by*: Lek d.d.

Pogodba št. I/8-106259/2008	Študij in analiza farmacevtskih materialov / *Studies and Analysis of Pharmaceutical Materials* Nosilec / *Principal Researcher*: J. Koller Financer / *Sponsored by*: Krka d.d.

MEDNARODNO SODELOVANJE NA PODROČJU IZOBRAŽEVANJA / INTERNATIONAL COOPERATION IN THE FIELD OF EDUCATION

- J. Dolenc, asistentka na Zvezni tehniški visoki šoli (ETH), Zürich, pri prof. dr. W. F. van Gunsternu / *Teaching Assistant at the ETH, Zürich (Prof. W. F. van Gunsteren)*
- V. Vlachy, 'adjunct' profesor na University of California, San Francisco Campus, ZDA (februar 2010) / *Adjunct Professor*, šest ur predavanj z naslovom: *Ions in Water: From Debye-Hückel Limiting Law to the Ion-Specific Effects (a Series of Lectures)*
- V. Vlachy, gostujoči profesor na Université Pierre et Marie Curie, Paris 6, Francija (april 2010) / *Visiting Professor*, šest ur predavanj z naslovom: *Ions in Water: From Debye-Hückel Limiting Law to Ion-Specific Effects in the Presence of Hydrophobic Groups (a Series of Lectures)*
- Č. Podlipnik, gostujoči raziskovalec na Univerzi v Milanu, junij 2010 / *Visiting Researcher at the University of Milano, June 2010*
- A. Godec, mentor slovenske srednješolske ekipe na mednarodni kemijski olimpijadi v Tokiu, Japonska, 2010 / *Mentor of the Slovenian Team at the International Chemistry Olympiad, Tokyo, Japan, 2010*
- Podiplomska študentka Jitka Krouská, Faculty of Chemistry, Brno University of Technology, Brno, Češka, februar – marec s štipendijo COST D43 in april – junij s štipendijo Erasmus, delovna mentorica: M. Bešter Rogač / *Visiting Postgraduate Student*
- Podiplomski študent Erik Gutierrez Valladares, Universidad Nacional Autónoma de México, Mehika, marec – junij 2010, delovna mentorja: V. Vlachy in B. Hribar Lee / *Visiting Postgraduate Student*

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

COST D–43	*Colloid and Interface Chemistry for Nanotechnology* Nosilka / *Principal Researcher:* M. Bešter Rogač
COST MP-0802	*Self-Assembled Guanosine Structures for Molecular Electronic Devices* Koordinator / *Coordinator:* J. Lah

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Avstrija *Slovenia – Austria*	Kontrolirano sproščanje funkcionalnih molekul iz nosilnih sistemov iz novih materialov / *Controlled Release of Functional Molecules from Carrier Systems Made from New Materials* Nosilec / *Principal Researcher:* M. Tomšič
Slovenija – ZDA (NIH) *Slovenia – USA* *(NIH Grant)*	Solvatacija v bioloških sistemih/ *Solvation in Biology* Nosilca / *Principal Researchers*: V. Vlachy, K. A. Dill (UC San Francisco)
Slovenija – ZDA *Slovenia – USA*	Modeli vode ter hidratacija preprostih in sestavljenih topljencev / *Models of Water and Hydration of Simple and Complex Solutes* Nosilec / *Principal Researcher*: V. Vlachy
Slovenija – Madžarska *Slovenia – Hungary*	Obravnava strukture kompleksnih tekočin z metodami sipanja in reverzno simulacijo Monte Carlo / *Understanding the Structure of Complex Liquids by Scattering Methods and Reverse Monte Carlo Simulation* Nosilec / *Principal Researcher:* A. Jamnik
Slovenija – Poljska *Slovenia – Poland*	Struktura in dinamika v kompleksnih nanostrukturiranih raztopinah / *Structure and Dynamics in Complex Nanostructured Solutions* Nosilec / *Principal Researcher:* A. Jamnik
Slovenija – Francija *Slovenia – France* BI-FR/09-10-PROTEUS-012	Raziskave interakcij površinsko aktivnih snovi z magnetnimi nanokoloidi v biološko sprejemljivih suspenzijah / *Study of the Interaction of Surfactants with Magnetic Nanocolloids in Biocompatible Suspensions* Nosilka / *Principal Researcher*: M. Bešter Rogač
Slovenija – Flandrija *Slovenia – Flanders*	Moduli toksin-antitoksin: Funkcija, struktura in termodinamika / *Toxin-Antitoxin Modules: Function, Structure and Thermodynamics* Nosilec / *Principal Researcher:* J. Lah

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

– Milko Novič, SENARC d.o.o., Ljubljana, Slovenija, Paul R. Haddad, Australian Centre for Research on Separation Science (ACROSS), School of Chemistry, University of Tasmania, Australia: Študij interakcij med dispergiranim polielektrolitom (popolnoma sulfonizirani stiren-divinilbenzen) in raztopljenim šibkim elektrolitom (šibka organska kislina) / *The Study of Interactions between Insoluble Fully Sulfonized and Completely Hydrated Polyelectrolyte and Dissolved Weak Electrolytes (Lower Fatty Acids)*, March 2010

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

FK1. KOGEJ, Ksenija. Association and structure formation in oppositely charged polyelectrolyte-surfactant mixtures. *Adv. colloid interface sci.*. [Print ed.], 2010, vol. 158, no. 1/2, str. 68–83. [COBISS.SI-ID 34100741]

FK2. CHESHEV, Pavel, MORELLI, Laura, MARCHESI, Marco, PODLIPNIK, Črtomir, BERGSTRÖM, Maria, BERNARDI, Anna. Synthesis and affinity evaluation of a small library of bidentate cholera toxin ligands : towards nonhydrolyzable ganglioside mimics. *Chemistry (Weinh., Print)*. [Print ed.], 2010, vol. 16, no. 6, str. 1951–1967. [COBISS.SI-ID 33990661]

FK3. YUAN-TAO, Xiang, JAMNIK, Andrej, KAI-WEI, Yang. Structural properties of effective potential model by liquid state theories. *Chinese physics. B*, 2010, vol. 19, no. 11, art. no. 110505 (9 str.). [COBISS.SI-ID 34662661]

FK4. RODRÍGUEZ-ABREU, Carlos, SANCHEZ-DOMÍNGUEZ, Margarita, ŠARAC, Bojan, BEŠTER-ROGAČ, Marija, SHRESTHA, Rekha Goswami, SHRESTHA, Lok Kumar, VARADE, Dharmesh, GHOSH, Goutam, ASWAL, Vinod K. Solution behavior of aqueous mixtures of low and high molecular weight hydrophobic amphiphiles. *Colloid polym. sci.*, 2010, vol. 288, no. 7, str. 739–751. [COBISS.SI-ID 33978373]

FK5. DE JONGE, Natalie, HOHLWEG, Walter, GARCIA-PINO, Abel, RESPONDEK, Michal, BUTS, Lieven, HAESAERTS, Sarah, LAH, Jurij, ZANGGER, Klaus, LORIS, Remy. Structural and thermodynamic characterization of Vibrio fischeri CcdB. *J Biol Chem*, 2010, vol. 285, no. 8, str. 5606–5613. [COBISS.SI-ID 33885957]

FK6. VLACHY, Vojko, HRIBAR, Barbara, BHUIYAN, Lutful B. Mean activity coefficient of a simple electrolyte, dissolved in the presence of an arbitrary number of cosolute components. *J. chem. eng. data*, 2010, issue 5, vol. 55, str. 1855–1859. [COBISS.SI-ID 33832197]

FK7. BEŠTER-ROGAČ, Marija, HUNGER, Johannes, STOPPA, Alexander, BUCHNER, Richard. Molar conductivities and association constants of 1-butyl-3-methylimidazolium chloride and 1-butyl-3-methylimidazolium tetrafluoroborate in methanol and DMSO. *J. chem. eng. data*, 2010, vol. 55, no. 5, str. 1799–1803. [COBISS.SI-ID 33313541]

FK8. BONČINA, Matjaž, APELBLAT, Alexander, BEŠTER-ROGAČ, Marija. Dilute aqueous solutions with formate ions : a conductometric study. *J. chem. eng. data*, 2010, vol. 55, no. 5, str. 1951–1957. [COBISS.SI-ID 33672709]

FK9. OUTHWAITE, C. W., BHUIYAN, Lutful B., VLACHY, Vojko, HRIBAR, Barbara. Activity coefficients of an electrolyte in a mixture with a high density neutral component. *J. chem. eng. data*, 2010, vol. 55, no. 10, str. 4248–4254. [COBISS.SI-ID 34507269]

FK10. URBIČ, Tomaž, DILL, Ken A. A statistical mechanical theory for a two-dimensional model of water. *J. chem. phys.*, 2010, vol. 132, no. 22, art. no. 224507 (9 str.). [COBISS.SI-ID 34425605]

FK11. LAJOVIC, Andrej, TOMŠIČ, Matija, JAMNIK, Andrej. The complemented system approach : a novel method for calculating the x-ray scattering from computer simulations. *J. chem. phys.*, 2010, vol. 133, no. 17, art. no. 174123 (6 str.).[COBISS.SI-ID 34580741]

FK12. PODLIPNIK, Črtomir, TUTINO, Federico, BERNARDI, Anna, SENECI, Pierfausto. DFG-in and DFG-out homology models of TrkB kinase receptor : induced-fit and ensemble docking. *J. mol. graph. model.*. [Print ed.], 2010, vol. 29, no. 3, str. 309–320. [COBISS.SI-ID 34621701]

FK13. BEŠTER-ROGAČ, Marija, KLOFUTAR, Cveto, RUDAN TASIČ, Darja. Association of hydrophobic ions in aqueous solution : a conductometric study of symmetrical tetraalkylammonium cyclohexylsulfamates. *J. mol. liq.*. [Print ed.], 2010, vol. 156, no. 1, str. 82–88. [COBISS.SI-ID 33979653]

FK14. TOPORIŠIČ, Rebeka, MLAKAR, Anita, HVALA, Jernej, PRISLAN, Iztok, ZUPANČIČ-KRALJ, Lucija. Identification of new impurities of enalapril maleate on oxidation in the presence of magnesium monoperoxyphthalate. *J. pharm. biomed. anal.*. [Print ed.], 2010, vol. 52, no. 2, str. 294–299. [COBISS.SI-ID 34108677]

FK15. TUTTLE, Tell, CERKOVNIK, Janez, KOLLER, Jože, PLESNIČAR, Božo. The search for protonated dihydrogen trioxide (HOOOH) : insights from theory and experiment. *J. phys. chem., A Mol. spectrosc. kinet. environ. gen. theory*, 2010, vol. 114, no. 30, str. 8003–8008. [COBISS.SI-ID 34295813]

FK16. BREN, Urban, LAH, Jurij, BREN, Matevž, MARTÍNEK, Václav, FLORIÁN, Jan. DNA duplex stability : the role of preorganized electrostatics. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2010, vol. 114, no. 8, str. 2876–2885. [COBISS.SI-ID 33744645]

FK17. BONČINA, Matjaž, LAH, Jurij, REŠČIČ, Jurij, VLACHY, Vojko. Thermodynamics of the lysozyme-salt interaction from calorimetric titrations. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2010, vol. 114, no. 12, str. 4313–4319. [COBISS.SI-ID 33831941]

FK18. DROBNAK, Igor, VESNAVER, Gorazd, LAH, Jurij. Model-based thermodynamic analysis of reversible unfolding processes. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2010, vol. 114, no. 26, str. 8713–8722. [COBISS.SI-ID 34219269]

FK19. LUKŠIČ, Miha, HRIBAR, Barbara, VLACHY, Vojko. Interplay of ion-specific and charge-density effects in aqueous solutions of weakly charged ionenes as revealed by electric-transport measurements. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2010, vol. 114, no. 32, str. 10401–10408. [COBISS.SI-ID 34322949]

FK20. HRIBAR, Barbara, DILL, Ken A., VLACHY, Vojko. Receptacle model of salting-in by tetramethylammonium ions. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2010, vol. 114, no. 46, str. 15085–15091. [COBISS.SI-ID 34600453]

FK21. VRHOVŠEK, Aleksander, GEREBEN, Orsolya, POTHOCZKY, Szilvia, TOMŠIČ, Matija, JAMNIK, Andrej, KOHARA, Shinji, PUSZTAI, László. An approach towards understanding the structure of complex molecular systems : the case of lower aliphatic alcohols. *J. phys., Condens. matter*, 2010, vol. 22, no. 40, art. no. 404214 (9 str.). [COBISS.SI-ID 34490373]

FK22. KALYUZHNYI, Yu. V., VLACHY, Vojko, DILL, Ken A. Aqueous alkali halide solutions : can osmotic coefficients be explained on the basis of the ionic sizes alone?. *PCCP. Phys. chem. chem. phys. (Print)*, 2010, vol. 12, no. 23, str. 6260–6266. [COBISS.SI-ID 34118149]

FK23. DRUCHOK, M., VLACHY, Vojko. Molecular dynamics study of the hydrophobic 6,6-ionene oligocation in aqueous solution with sodium halides. *Pure appl. chem.*, 2010, vol. 82, no. 10, str. 1943–1955. [COBISS.SI-ID 34400005]

FK24. BEŠTER-ROGAČ, Marija, KLOFUTAR, Cveto, RUDAN TASIČ, Darja. Osmotic coefficient of aqueous solutions of cyclohexylsulfamic acid at the freezing point of solutions. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 4, str. 849–854. [COBISS.SI-ID 34669573]

FK25. GODEC, Andrej. Tri bronaste medalje na kemijski olimpiadi v Deželi vzhajajočega sonca. *Kemija v šoli in družbi*, 2010, letn. 22, št. 3, str. 28–33. [COBISS.SI-ID 34752773]

FK26. GODEC, Andrej. Kemijska olimpiada 2010 v Tokyu. *Acta chim. slov.*. [Tiskana izd.], 2010, letn. 57, št. Suppl., str. S63–S65. [COBISS.SI-ID 34555397]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

FK27. VLACHY, Vojko. Polyelectrolytes in water: how the presence of hydrophobic groups modifies the ion-specific effects : [keynote lecture]. V: 28th Annual Meeting MLG, September 5–9, 2010, Lviv, Ukraine. *Programme & abstracts : complex liquids : modern trends in exploration, understanding and application.* Lviv: Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 2010, str. 27. [COBISS.SI-ID 34429957]

FK28. KALYUZHNYI, Yu. V., VLACHY, Vojko, DILL, Ken A. Aqueous alkali halide solutions: can osmotic coefficients be explained on the basis of the ionic sizes alone? : [plenary lecture]. V: 28th Annual Meeting MLG, September 5–9, 2010, Lviv, Ukraine. *Programme & abstracts : complex liquids : modern trends in exploration, understanding and application*. Lviv: Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 2010, str. 43. [COBISS.SI-ID 34430213]

FK29. BEŠTER-ROGAČ, Marija. Raztopine elektrolitov – izziv ali zgodovina = Electrolyte solutions – a challenge or old news : [uvodno sekcijsko predavanje]. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–9. [COBISS.SI-ID 34463237]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

FK30. ČEBAŠEK, Sašo, LUKŠIČ, Miha, POHAR, Ciril, VLACHY, Vojko. Razredčilne entalpije vodnih raztopin 3,3-; 4,5-; 6,6- in 6, 9-ionen fluoridov in jodidov = Heats of dilution of aqueous solutions of 3,3-; 4,5-; 6,6- and 6,9-ionene fluorides and iodides. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–7. [COBISS.SI-ID 34464773]

FK31. PRELESNIK, Simona, HANSSON, Per, KOGEJ, Ksenija. Fazni diagram in strukture v mešanicah anionskega polielektrolita, kationskega surfaktanta in vode = Phase diagram and structures in anionic polyelectrolyte, cationic surfactant and water mixtures. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–10. [COBISS.SI-ID 34465285]

FK32. KROFLIČ, Ana, ŠARAC, Bojan, BEŠTER-ROGAČ, Marija. Vpliv temperature in dodanega elektrolita na termodinamiko micelizacije alkiltrimetilamonijevih kloridov = Temperature and salt-induced micellization of alkyltrimethylammonium chlorides: a thermodynamic study. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–11. [COBISS.SI-ID 34463493]

FK33. PODLIPNIK, Črtomir, SENECI, Pierfausto. Strukturni elementi receptorjev Trk in smernice za razvoj njihovih inhibitorjev = Structural elements of Trk receptors and directives for development of their inhibitors. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–17. [COBISS.SI-ID 34465797]

OBJAVLJENI POVZETEK ZNANSTVENEGA PRISPEVKA NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION ABSTRACT (INVITED LECTURE)

FK34. DROBNAK, Igor, LAH, Jurij. The molecular and functional origins of picomolar binding affinity of an intrinsically disordered protein domain : [invited lecture]. V: *24th Annual Gibbs Conference on Biothermodynamics : Tauch of Nature Conference Center Southern Illinois University Carbondale, Illinois, September 25–28, 2010*. [S. l.: s. n.], 2010, str. 31. [COBISS.SI-ID 34676229]

SAMOSTOJNI ZNANSTVENI SESTAVEK ALI POGLAVJE V MONOGRAFSKI PUBLIKACIJI / INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

FK35. TOMŠIČ, Matija, GLATTER, Otto. From bulk to dispersed hierarchically organized lipid phase systems. V: IGLIČ, Aleš (ur.). *Advances in planar lipid bilayers and liposomes : volume 12*, (Advances in planar lipid bilayers and liposomes). Amsterdam; Elsevier: Academic Press, cop. 2010, str. 167–200. [COBISS.SI-ID 34569221]

UNIVERZITETNI ALI VISOKOŠOLSKI UČBENIK Z RECENZIJO / REVIEWED UNIVERSITY AND ACADEMIC TEXTBOOK

FK36. KOGEJ, Ksenija. *Površinska in koloidna kemija*. 1. izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. IX, 185 str., ilustr. ISBN 978-961-6756-15-0. [COBISS.SI-ID 251129600]

FK37. KOLLER, Jože. *Struktura atomov in molekul : (bolonjski program) : visokošolski učbenik*. 1. izd. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 209 str., ilustr. ISBN 978-961-6756-21-1. [COBISS.SI-ID 252887296]

FK38. KOLLER, Jože. *Struktura atomov in molekul, Molekule, osnove spektroskopije : visokošolski učbenik*. [Ponatis]. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 114 str., ilustr. ISBN 978-961-6286-21-3. [COBISS.SI-ID 253008384]

FK39. KOLLER, Jože. *Struktura atomov in molekul, Osnove kvantne mehanike, atomi : visokošolski učbenik*. [Ponatis]. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 117 str., ilustr. ISBN 978-961-6756-22-8. [COBISS.SI-ID 253269760]

FK40. KOLLER, Jože. *Struktura atomov in molekul, Zbirka nalog z rešitvami : visokošolski učbenik*. [Ponatis]. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2010. 121 str., ilustr. ISBN 978-961-6286-05-3. [COBISS.SI-ID 253008640]

SREDNJEŠOLSKI, OSNOVNOŠOLSKI ALI DRUGI UČBENIK Z RECENZIJO / REVIEWED SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK

FK41. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Il mio primo approccio alla chimica 1 : chimica per la classe VIII della scuola elementare, Quaderno attivo*. 4a ed. Ljubljana: Modrijan, 2010. 116 str., ilustr. ISBN 978-961-241-193-0. [COBISS.SI-ID 251249920]

FK42. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Il mio primo approccio alla chimica 2 : chimica per la classe IX della scuola elementare, Quaderno attivo*. 3a ed. Ljubljana: Modrijan, 2010. ISBN 978-961-241-236-4. [COBISS.SI-ID 251342848]

FK43. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Moja prva kemija 2 : kemija za 9. razred dvojezične osnovne šole = Első kémiám 2 : kémia a kétnyelvű általános iskola 9. osztálya számára*. 2. izd. Ljubljana: Modrijan, 2010. 2 zv. (112, 112 str.), ilustr. ISBN 978-961-241-099-5. ISBN 978-961-241-100-8. [COBISS.SI-ID 251402240]

FK44. GODEC, Andrej, LEBAN, Ivan. *Kemijske reakcije : učbenik za kemijo v gimnaziji*. 1. izd. Ljubljana: Modrijan, 2010. 175 str., ilustr. ISBN 978-961-241-422-1. [COBISS.SI-ID 250443520]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

FK45. BONČINA, Matjaž, CERAR, Janez, HRIBAR, Barbara, LAH, Jurij, LAJOVIC, Andrej, LUKŠIČ, Miha, PRISLAN, Iztok. *Laboratorijske vaje iz fizikalne kemije za študente farmacije : študijsko leto 2009/2010*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za fizikalno kemijo, 2010. 72 str., graf. prikazi. [COBISS.SI-ID 33741573]

FK46. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Moja prva kemija 1 : kemija za 8. razred osnovne šole, Delovni zvezek*. 7. izd. Ljubljana: Modrijan, 2010. 116 str., ilustr. ISBN 978-961-6465-82-3. [COBISS.SI-ID 249880576]

FK47. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Moja prva kemija 2 : kemija za 9. razred osnovne šole, Delovni zvezek*. 5. izd. Ljubljana: Modrijan, 2010. 96 str., ilustr. ISBN 978-961-241-045-2. [COBISS.SI-ID 249880832]

PATENTNA PRIJAVA / PATENT APPLICATION

FK48. BEŠTER-ROGAČ, Marija. *Sistem za določanje dielektrične konstante topil : št. P-201000136*. Ljubljana: Urad Republike Slovenije za intelekturalno lastnino, 15. 9. 2010. [COBISS.SI-ID 34485509]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

FK49. LAH, Jurij, DROBNAK, Igor. Bacterial toxin-antitoxin modules: thermodynamics of interactions governing functionality of the ccd module : University of Nebraska Medical Center, Department of Pharmaceutical Sciences, Friday, September 24, 2010. 2010; Omaha. [COBISS.SI-ID 34672901]

FK50. LUKŠIČ, Miha. How does the charge density of cationic polyelectrolytes (ionenes) in water influence the ion-specific effects : experimental evidences supplemented with simulations and classical polyelectrolyte theories : [vabljeno predavanje] : Universidad Nacional Autónoma de México, Instituto de Quimica, Mexico City, Mexico. Mexico City, 2010. [COBISS.SI-ID 34625029]

FK51. VLACHY, Vojko. How the interplay of hydrophobic and Coulomb interaction shapes the properties of polyelectrolyte solutions : [University of Helsinki, Monday, June 14th, 2010]. Helsinki, 2010. [COBISS.SI-ID 34163973]

FK52. VLACHY, Vojko. The ion-specific effects in presence of hydrophobic groups : [Commissariat à l'Énergie Atomique (CEA) Saclay, Paris, France, 16. 4. 2010]. Paris, 2010. [COBISS.SI-ID 34007045]

FK53. VLACHY, Vojko. Ions in water: from Debye-Huckel limiting law to ion-specific effects in presence of hydrophobic groups : [University Pierre et Marie Curie, Paris, France, 12. 4. – 13. 4. 2010]. Paris, 2010. [COBISS.SI-ID 34006789]

FK54. VLACHY, Vojko. Ions in water: from Debye-Huckel limiting law to the ion-specific effects : [University of California, San Francisco, 3. 2. – 4. 2. 2010]. San Francisco, 2010. [COBISS.SI-ID 34006533]

FK55. TOMŠIČ, Matija. Simple alcohols in microemulsion systems of nonionic surfactant and their structure in bulk : SAXS, DLS and Monte Carlo studies : Division of Physical Chemistry, Center of Chemistry and Chemical Engineering, Lund University, Lund, February 10, 2010. 2010; Lund. [COBISS.SI-ID 33723909]

UREDNIK / EDITORSHIP

FK56. *Acta chimica slovenica*. Vesnaver, Gorazd (član uredniškega odbora 1998–), Bešter-Rogač, Marija (področna urednica 2003–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [COBISS.SI-ID 14086149]

FK57. *Journal of molecular liquids*. Bešter-Rogač, Marija (član uredniškega odbora 2008–). [Print ed.]. Amsterdam: Elsevier. ISSN 0167-7322. [COBISS.SI-ID 15382277]

FK58. GERLIČ, Ivan, GOLOB, Nika, FERK SAVEC, Vesna, KRNEL, Dušan, MAJER, Janja, ŽARIĆ, Kornelia, GODEC, Andrej, DEVETAK, Iztok, FERK, Eva, DOJER, Brina, SIKOŠEK, Darinka. *Didaktična gradiva/modeli : (kemijske vsebine) : K3 : projekt: Razvoj naravoslovnih kompetenc : (01. 01. 2010–31. 03. 2010)*. Maribor: Fakulteta za naravoslovje in matematiko, 2010. 336 str., ilustr. [COBISS.SI-ID 17628680]

KATEDRA ZA ORGANSKO KEMIJO
CHAIR OF ORGANIC CHEMISTRY

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Boris Šket

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Marijan Kočevar
izr. prof. dr. Janez Košmrlj
prof. dr. Andrej Petrič
prof. dr. Božo Plesničar, zaslužni profesor (upokojen) / *Professor Emeritus*
prof. dr. Slovenko Polanc
akademik prof. dr. Branko Stanovnik
prof. dr. Jurij Svete
prof. dr. Boris Šket
akademik prof. dr. Miha Tišler, zaslužni profesor (upokojen) / *Professor Emeritus*
izr. prof. dr. Bojan Verček
prof. dr. Marko Zupan

Asistenti / Assistants
doc. dr. Janez Cerkovnik
izr. prof. dr. Darko Dolenc
doc. dr. Marjan Jereb
dr. Berta Košmrlj
doc. dr. Franci Kovač
doc. dr. Franc Požgan
doc. dr. Bogdan Štefane

Raziskovalci / Researchers
dr. Uroš Grošelj
dr. Krištof Kranjc
Nenad Maraš, univ. dipl. kem.
dr. Jernej Wagger
dr. Damijana Urankar

Tehniki / Technicians
Zdenka Kadunc
Tončka Kozamernik
Branka Miklavčič
Irena Povalej
Zdenka Sakelšek
Tatjana Stipanović

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Jernej Baškovč	B. Stanovnik	2007–2012	doktorski študij / *PhD*
Jure Bezenšek	B. Stanovnik	2009–2013	doktorski študij / *PhD*
Vita Majce	S. Polanc	2007–2012	doktorski študij / *PhD*
Bojan Burja	S. Polanc	2005–2010	doktorski študij / *PhD*
Petra Galer	B. Šket	2009–2013	doktorski študij / *PhD*
Martin Gazvoda	S. Polanc	2009–2013	doktorski študij / *PhD*
Jure Hren	M. Kočevar	2006–2011	doktorski študij / *PhD*
Amadej Juranovič	M. Kočevar	2008–2012	doktorski študij / *PhD*
Marko Krivec	M. Kočevar	2010–2014	doktorski študij / *PhD*
Črt Malavašič	J. Svete	2007–2011	doktorski študij / *PhD*
Ana Novak	J. Svete	2009–2013	doktorski študij / *PhD*

Ostali podiplomski študenti, ki niso v rednem delovnem razmerju /
Other Postgraduate Students
Sanja Čavar
Žiga Nose

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemija / *Chemistry* – UN:
Organska kemija I / *Organic Chemistry I*

Biokemija / *Biochemistry* – UN:
Organska kemija I, II / *Organic Chemistry I, II*

Kemijsko inženirstvo / *Chemical Engineering* – UN:
Organska kemija / *Organic Chemistry*

Tehniška varnost / *Technical Safety* – UN:
Kemija / *Chemistry*

Kemijska tehnologija / *Chemical Technology* – VS:
Organska kemija I, II / *Organic Chemistry I, II*
Praktikum iz kemije I / *Practicals in Chemistry I*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Organska kemija / *Organic Chemistry* – UN
Organska kemija II / *Organic Chemistry II* – UN
Organska kemija / *Organic Chemistry* – VS
Organska analiza / *Organic Analysis* – UN
Spektroskopske metode / *Spectroscopic Methods* – UN
Analitika in spektroskopija / *Analysis and Spectroscopy* – VS
Kemija heterocikličnih spojin / *Chemistry of Heterocyclic Compounds* – UN
Načrtovanje organskih sintez / *Planning of Organic Syntheses* – UN
Izbrana poglavja iz organske kemije / *Selected Topics in Organic Chemistry* – UN
Organska kemija biološko pomembnih spojin / *Organic Chemistry of Biologically Importnat Compounds* – UN
Bioorganska kemija / *Bioorganic Chemistry* – UN
Usmerjena organska sinteza / *Directed Organic Synthesis* – UN
Bioaktivne spojine / *Bioactive Compounds* – UN
Pretvorbe bioaktivnih spojin / *Transformations of Bioactive Compounds* – UN
Nukleinske kisline in polinukleotidi / *Nucleic Acids and Polynucleotides* – UN
Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UN
Poskusi v organski kemiji / *Experiments in Organic Chemistry* – UN

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Izbrana poglavja iz organske kemije / *Selected Topics in Organic Chemistry*
Izbrana poglavja iz heterociklične kemije / *Selected Topics in Heterocyclic Chemistry*
Študij mehanizmov transformacij organskih spojin / *Studies of Organic Transformation Mechanisms*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Organska kemija / *Organic Chemistry* FFA – UN

Splošna in organska kemija / *General and Organic Chemistry* FFA – UN

Organska kemija / *Organic Chemistry* BF – UN

Teoretske osnove tiskarskih procesov / *Fundamental Theoretical Principles of Printing Processes* NTF – UN

Kemija II / *Chemistry II* NTF – VS

Kemija / *Chemistry* PEF – UN

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Organska kemija / *Organic Chemistry* PEF – UN

Organska kemija / *Organic Chemistry* BF – UN

Kemija organskih materialov / *Chemistry of Organic Materials* NTF – UN

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

- Sinteza novih reagentov na osnovi 3-dimetilaminopropenoatov in sorodnih enaminov ter aplikacija teh spojin za sintezo novih heterocikličnih sistemov / *Synthesis of New Reagents Based on 3-Dimethylaminopropenoates and Related Enamines and their Application in the Synthesis of New Heterocyclic Systems*
- Sinteza naravnih spojin in njihovih analogov z enaminsko metodologijo / *Synthesis of Natural Products and their Analogues Using the Enamine Methodology*
- Sinteza in transformacije kiralnih spojin / *Synthesis and Transformations of Chiral Compounds*
- 1,3-Dipolarne cikloadicije / *1,3-Dipolar Cycloadditions*
- Stereoselektivna sinteza / *Stereoselective Synthesis*
- Sinteza heterocikličnih analogov peptidov / *Synthesis of Heterocyclic Analogues of Peptides*
- Kombinatorna in paralelna sinteza / *Combinatorial and Parallel Synthesis*
- Organokataliza / *Organocatalysis*
- Načrtovanje in sinteza spojin z antimalarijsko aktivnostjo / *Design and Synthesis of Compounds with Antimalarial Activity*
- Novi pristopi k sintezi antibakterijsko aktivnih molekul / *New Approaches towards the Synthesis of Molecules with Antibacterial Activity*
- Sinteza in evalvacija novih potencialnih citostatikov diazenskega tipa / *Synthesis and Evaluation of Novel Potential Diazene-Type Cytostatic Agents*
- Inovativna kataliza: novi procesi in selektivnost / *Innovative Catalysis: New Processes and Selectivities*
- Reakcije pod mikrovalovi in visokimi pritiski / *Microwave-Assisted Reactions and Reactions under High-Pressure*
- Študij halogeniranja organskih molekul, novi reagenti, novi pristopi / *Studies on Halogenation of Organic Compounds, New Reagents, and New Approaches*
- Raziskave reakcijskih pogojev za organske transformacije / *Studies on the Reaction Conditions for Organic Transformations*

- Priprava in uporaba imobiliziranih (polimernih) reagentov / *Preparation and Application of Immobilized (Polymeric) Reagents*
- Študij mehanizmov oksidacij organskih spojin / *Studies on the Oxidation Mechanisms of Organic Compounds*
- Študij mehanizmov fototransformacij organskih halogenidov / *Studies on the Mechanisms of Phototransformation of Halogenated Organic Compounds*
- Sinteza in karakterizacija molekularnih sond za medicinske raziskave / *Synthesis and Characterization of Molecular Probes for Medical Research*
- Izomerni »Klik« ligandi za komplekse kovin prehoda / *Isomeric »Click« Ligands For Transition Metal Complexes*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- M. Kočevar: 2010– »IUPAC Fellow« (http://www.iupac.org/web/per/kocevar) / *IUPAC Fellow since 2010– (http://www.iupac.org/web/per/kocevar)*
- A. Novak (soavtorji: Uroš Grošelj, Jure Bezenšek, Katarina Stare, Branko Stanovnik, Jurij Svete): Nagrada za najboljši poster (za mlade raziskovalce): »Synthesis and Structure of Heterocyclic Peptides with Variable Configuration«; XXIVth European Colloquium on Heterocyclic Chemistry, 23.–27. Avgust, Dunaj, Avstrija [COBISS.SI-ID 34404357] / *Poster Prize (for Young Researchers), XXIVth European Colloquium on Heterocyclic Chemistry, August 23–27, 2010, Vienna. "Synthesis and Structure of Heterocyclic Peptides with Variable Configuration" (Co-authors: Uroš Grošelj, Jure Bezenšek, Katarina Stare, Branko Stanovnik, Jurij Svete). [COBISS.SI-ID 34404357]*
- B. Stanovnik: Zlati znak (Gold Badge) Fundacije za mednarodno znanstveno partnerstvo za prispevek k svetovni znanosti in mednarodnemu znanstvenemu sodelovanju (Sankt Peterburg 2010) / *Gold Badge of International Scientific Partnership Foundation for Contribution to World Science and International Scientific Collaboration (Sankt Peterburg 2010)*
- B. Stanovnik, Priznanje Krke d.o.o. ob 40-letnici Krkinih nagrad za izjemen prispevek pri usmerjanju in spodbujanju mladih k raziskovalnemu delu / *On the Occasion of 40th Anniversary of KRKA Awards an Award for the Exceptional Contribution to the Ecouragement of Young People for Reserach*
- M. Gazvoda, Prešernova nagrada FKKT za leto 2010 (mentor M. Kočevar) / *The Faculty Prešeren Award for 2010*
- P. Perdih, Prešernova nagrada FKKT za leto 2010 (mentor J. Svete) / *The Faculty Prešeren Award for 2010*
- J. Svete, pohvala Študentskega sveta za pedagoško delo na smeri Kemijska tehnologija / *Students Award for the Quality of Teaching in Chemical Technology Study Programme*

ČLANSTVO V AKADEMIJAH / MEMBERSHIP IN ACADEMIES

- M. Tišler, redni član Slovenske akademije znanosti in umetnosti / *Full Member, Slovenian Academy of Sciences and Arts*

– B. Stanovnik, redni član Slovenske akademije znanosti in umetnosti / *Full Member, Slovenian Academy of Sciences and Arts*
– M. Tišler, član Evropske akademije znanosti in umetnosti / *Member, European Academy of Sciences and Arts*
– B. Stanovnik, član Evropske akademije znanosti in umetnosti / *Member, European Academy of Sciences and Arts*
– J. Svete, član Evropske akademije znanosti in umetnosti / *Member, European Academy of Sciences and Arts*

DRUGO / OTHER

– M. Kočevar je član upravnega odbora *(member of the Steering Committee)* COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011).
– M. Kočevar: na povabilo predsednika IUPAC profesorja Jun-Il Jina je M. Kočevar z letom 2010 postal IUPAC Fellow (Glej: http://www.iupac.org/web/per/kocevar).
– B. Stanovnik je član senata za akreditacijo pri Svetu Republike Slovenije za visoko šolstvo (od 2007) / *Member of the Senate for Accreditation, The Council for Higher Education of the Republic of Slovenia (since 2007)*
– B. Stanovnik:
  a) Member of the Scientific Committee, European Colloquia of Heterocyclic Chemistry
  b) Member of the Scientific Committee, Blue Danube Symposia of Heterocyclic Chemistry
  c) Member of the Board of Electronic Journal ARKIVOC
  d) Member of the Advisory Board, Advances in Heterocyclic Chemistry
  e) Member of the Scientific Committee, TRAMECH Transmediterranean Symposia on Heterocyclic Chemistry
  f) Member of International Advisory Committee of the IBN SINA International Conferences on Pure and Applied Heterocyclic Chemistry
  g) Member of the Scientific Committee of Eurasian Meetings on Heterocyclic Chemistry
  h) Member of the Advisory Board, Trends in Heterocyclic Chemistry
  i) Head of the Unit for International Cooperation and Scientific Coordination, Slovenian Academy of Sciences and Arts, Ljubljana, Slovenia
  j) Dean of the Class for Natural Sciences, European Academy of Sciences and Arts, Salzburg, Austria and legat EASA for Slovenia for the period 2010–2014
  k) 1998–2004 Member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons, Den Haag, The Netherlands
  l) Member of the Advisory Board, Croatica Chemica Acta

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

– C, H, N – Analizator Perkin-Elmer 2400 II / *C, H, N – Analyzer Perkin Elmer 2400 II*
– UV – visible spektrofotometer Varian / *UV – Visible Spectrophotometer Varian*
– IR spektrometer BIO-RAD / *IR Spectrometer BIO-RAD*
– IR spektrometer Spectrum BX FTIR Perkin-Elmer / *IR Spectrometer Spectrum BX FTIR Perkin-Elmer*
– Polarimeter Perkin-Elmer / *Polarimeter Perkin-Elmer*

- Destilacijska aparatura Fisher-Jones / *Distillation Apparatus Fisher-Jones*
- Mettler-Toledo miniblock paralelni sintetizator – 12 pozicij / *Mettler-Toledo Miniblock Parallel Synthesizer – 12 Positions*
- Carousel reaction station paralelni sintetizator – 6 pozicij / *Carousel Reaction Station Paralel Synthesizer – 6 Positions*
- Büchi Syncore Polyvap+Reactor paralelni sintetizator in uparjevalnik– 24 pozicij / *Büchi Syncore Polyvap+Reactor Parallel Syntesizer and Evaporator – 24 Positions*
- Hettlab IR-Dancer Infra-Red Vortex evaporator (paralelni uparjevalnik) – 48 pozicij / *Hettlab IR-Dancer Infra-Red Vortex Evaporator (Parallel Evaporator) – 48 Positions*
- Starfish – multiexperiment work station / *Starfish – Multiexperiment Work Station*
- Laboratorijski mikrovalovni reaktor CEM / *Laboratory Microwave Reactor CEM*
- MPLC – preparativni kromatograf Büchi / *MPLC –Preparative Chromatograph Büchi*
- Aparatura za delo pod visokimi pritiski U 101 / *High-Pressure Reactor U 101*
- GC – Hewlett Packard HPG 890 Series / *GC – Hewlett Packard HPG 890 Series*
- Fotokemijski reaktor Buckinghamshire model MLU/8 / *Photochemical Reactor Buckinghamshire Model MLU/8*
- NMR spektrometer – Bruker Avance DPX 300 / *NMR Spectrometer – Bruker Avance DPX 300*
- Ozonator Welsbach model T-816 / *Ozonator Welsbach Model T-816*
- GC/MS Hewlett Packard 6890 / *GC/MS Hewlett Packard 6890*
- MS Micromass Platform II / *MS Micromass Platform II*
- Potopni hladilnik do –60 °C / *Cooler –60 °C*
- Hidrogenator Parr / *Parr Hydrogenator*
- Avtoklavi Berghof / *Autoclaves Berghof*
- Rotavaporji Büchi / *Rotavapors Büchi*
- Rotavapor Heidolph / *Rotavapor Heidolph*
- OptiMelt EZ (Stanford Scientific) – sistem za avtomatsko določevanje tališča / *OptiMelt EZ (Stanford Scientific) Automated Melting Point System*

SODELOVANJE V CENTRIH ODLIČNOSTI / CENTERS OF EXCELLENCE

Center odličnosti: EN-FIST – raziskave na področju zdravja, znanosti o življenju in naprednih novih materialov / *Center of Excellence: Multidisciplinary Research in Life Sciences and Advanced New Materials*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P1–0179 Sinteze in transformacije organskih spojin. Novi reagenti v stereoselektivni in regioselektivni sintezi aminokislin kot intermediatov v

organski sintezi / *Syntheses and Transformations of Organic Compounds. New Reagents in Stereoselective and Regioselective Synthesis of Amino Acids as Intermediates in Organic Synthesis*
Nosilec / *Principal Researcher:* B. Stanovnik

P1–0230 Organska kemija: Sinteza, struktura in aplikacija / *Organic Chemistry: Synthesis, Structure, and Application*
Nosilec / *Principal Researcher:* M. Kočevar

TEMELJNI PROJEKTI / BASIC RESEARCH

J1–6254 Reaktivni intermediati pri transformacijah organskih spojin / *Reactive Intermediates in the Transformation of Organic Compounds*
Nosilec / *Principal Researcher:* B. Šket

J1–6689 Sinteza heterocikličnih analogov aminokislin in peptidov / *Synthesis of Heterocyclic Analogs of Amino Acids and Peptides*
Nosilec / *Principal Researcher:* B. Stanovnik

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

Pogodba o sodelovanju: Sinteza titanovega kompleksa / *Cooperation Agreement: Synthesis of a Titanum Complex*
Nosilec / *Principal Researcher:* J. Košmrlj
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju: Sinteza 1,2-disubstituiranih tetrahidronaftalenskih derivatov / *Cooperation Agreement: Synthesis of 1,2-Disubstituted Tetrahydronaphthalene Derivatives*
Nosilec / *Principal Researcher:* J. Košmrlj
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju: Sinteza in pretvorba organoborovih spojin / *Cooperation Agreement: Synthesis and Transformation of Some Organoboron Compounds*
Nosilec / *Principal Researcher:* J. Košmrlj
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* M. Kočevar
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* B. Stanovnik
Financer / *Sponsored by:* Krka d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* J. Svete
Financer / *Sponsored by:* Boehringer-Ingelheim Pharma, Biberach, Nemčija

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Argentina *Slovenia – Argentina*	Funkcionalizacija izbranih organskih substratov in razvoj strategij za trajnostno organsko sintezo / *Functionalization of Selected Organic Substrates and Development of Strategies for a Sustainable Organic Synthesis* Nosilec / *Principal Researcher*: S. Polanc
Slovenija – Romunija *Slovenia – Romania*	Sinteza in katalitsko hidrogeniranje prokiralnih nenasičenih aminokislin / *Synthesis and Catalytic Hydrogenation of Prochiral Unsaturated Amino Acids* Nosilec / *Principal Investigator*: M. Kočevar
Slovenija – Češka *Slovenia – Czech Republic*	Nov pristop k antibakterijsko aktivnim molekulam / *New Approach to Antibacterial Active Molecules* Nosilec / *Principal Researcher:* S. Polanc

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

- C. Oliver Kappe, Christian Doppler Laboratory for Microwave Chemistry and Institute of Chemistry, Karl-Franzens-University Graz, Graz, Austria: *Microwave-Assisted Organic Synthesis. From Laboratory Curiosity to Standard Practice in 25 Years*, March 2010.
- Thomas Carell, Chair for Organic Chemistry I, LMU Munich, Department for Chemistry and Biochemistry, Munich, Germany: *The Chemistry of Genome Maintenance*, May 2010.
- Dieter E. Kaufmann, Institut für Organische Chemie, Technische Universität Clausthal, Clausthal-Zellerfeld: *The Value of Aryl Boranes. From Catalysis to Luminescence*, June 2010.
- Saverio Florio, Vice-Presidente della Societa Chimica Italiana, Dipartimento Farmaco-Chimico, Facolta di Farmacia, Universita di Bari, Bari, Italia: *α-Heteroaryl Substituted Organolithiums: Swinging Between Carbanions and Carbenoids*, September 2010.
- George J.P. Britovsek, Department of Chemistry, Imperial College London, UK: *Towards Green Oxidation with H_2O_2 and Non-Heme Iron Catalysts*, November 2010.

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

OK1. MARAŠ, Nenad, POLANC, Slovenko, KOČEVAR, Marijan. Synthesis of aryl alkyl ethers by alkylation of phenols with quaternary ammonium salts. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 29–36. http://acta.chem-soc.si/57/57-1-029.pdf. [COBISS.SI-ID 33795589]

OK2. BURJA, Bojan, ČIMBORA, Tamara, TOMIĆ, Sanja, JELUŠIĆ, Tihana, KOČEVAR, Marijan, POLANC, Slovenko, OSMAK, Maja. Pyrazolone-fused combretastatins and their precursors : synthesis, cytotoxicity, antitubulin activity and molecular modeling studies. *Bioorg. med. chem.*. [Print ed.], 2010, vol. 18, no. 7, str. 2375–2387, doi: 10.1016/j.bmc.2010.03.006. [COBISS.SI-ID 33791237]

OK3. ŠTEFANE, Bogdan, PERDIH, Andrej, PEVEC, Andrej, ŠOLMAJER, Tomaž, KOČEVAR, Marijan. The participation of 2H-pyran-2-ones in [4+2] cycloadditions : an experimental and computational study. *European journal of organic chemistry*, 2010, vol. 2010, issue 30, str. 5870–5883, doi: 10.1002/ejoc.201000236. [COBISS.SI-ID 34399749]

OK4. POŽGAN, Franc, LUKMAN, Klavdija, KOČEVAR, Marijan. An efficient synthesis of methyl esters of heterocyclic [alpha], [beta]-didehydro-[alpha]-amino acid derivatives. *Heterocycles*, 2010, vol. 82, no. 1, str. 543–554, doi: 10.3987/COM-10-S(E)25. [COBISS.SI-ID 34690821]

OK5. WANG, Jingxin, ŠTEFANE, Bogdan, JABER, Deana, SMITH, Jacqueline A. I., VICKERY, Christopher, DIOP, Mouhamed, SINTIM, Herman O. Remote C-H functionalization : using the N-O moiety as a atom-economical tether to obtain 1,5- and the rare 1,7-C-H insertions. *Angew. Chem. (Int. ed., Print)*. [Print ed.], 2010, vol. 49, no. 23, str. 3964–3968, doi: 10.1002/anie.201000160. [COBISS.SI-ID 34061573]

OK6. SOSIČ, Izidor, ŠTEFANE, Bogdan, KOVAČ, Andreja, TURK, Samo, BLANOT, Didier, GOBEC, Stanislav. The synthesis of novel 2,4,6-trisubstituted 1, 3,5-triazines: a search for potential MurF enzyme inhibitors. *Heterocycles*, 2010, vol. 81, no. 1, str. 91–115. http://www.docin.com/p-48736457.html. [COBISS.SI-ID 2791793]

OK7. ŠTEFANE, Bogdan. Selective addition of organolithium reagents to BF[sub]2-chelates of [beta]-ketoesters. *Org. lett.*, 2010, vol. 12, no. 13, str. 2900–2903, doi: 10.1021/ol100620j. [COBISS.SI-ID 34162181]

OK8. ROGER, Julien, POŽGAN, Franc, DOUCET, Henri. Palladium-catalysed direct arylation of heteroaromatics bearing unprotected hydroxyalkyl functions using aryl bromides. *Advanced Synthesis & Catalysis*. [Print ed.], 2010, vol. 352, no. 4, str. 696–710, doi: 10.1002/adsc.200900793. [COBISS.SI-ID 33849861]

OK9. KIMMEL, Roman, KAFKA, Stanislav, KOŠMRLJ, Janez. Selective formation of glycosidic linkages of N-unsubstituted 4-hydroxyquinolin-2-(1H)-ones. *Carbohydr. res.*. [Print ed.], 2010, vol. 345, no. 6, str. 768–779, doi: 10.1016/j.carres.2010.01.023. [COBISS.SI-ID 33829381]

OK10. URANKAR, Damijana, PEVEC, Andrej, TUREL, Iztok, KOŠMRLJ, Janez. Pyridyl conjugated 1,2,3-triazole is a versatile coordination ability ligand enabling supramolecular associations. *Cryst. growth des.*, 2010, vol. 10, no. 11, str. 4920–4927, doi: 10.1021/cg100993k. [COBISS.SI-ID 34469381]

OK11. URANKAR, Damijana, PINTER, Balazs, PEVEC, Andrej, DE PROFT, Frank, TUREL, Iztok, KOŠMRLJ, Janez. Click-triazole N2 coordination to transition-metal ions is assisted by a pendant pyridine substituent. *Inorg. chem.*, 2010, vol. 49, no. 11, str. 4820–4829, doi: 10.1021/ic902354e. [COBISS.SI-ID 34066949]

OK12. URANKAR, Damijana, KOŠMRLJ, Janez. Preparation of diazenecarboxamide-carboplatin conjugates by click chemistry. *Inorg. Chim. Acta*. [Print ed.], 2010, vol. 363, no. 14, str. 3817–3822, doi: 10.1016/j.ica.2010.07.031. [COBISS.SI-ID 34469125]

OK13. ČASAR, Zdenko, STEINBÜCHER, Miha, KOŠMRLJ, Janez. Lactone pathway to statins utilizing the Wittig reaction. The synthesis of rosuvastatin. *J. org. chem.*, 2010, vol. 75, no. 19, str. 6681–6684, doi: 10.1021/jo101050z. [COBISS.SI-ID 34441989]

OK14. URANKAR, Damijana, STEINBÜCHER, Miha, KOSJEK, Jaka, KOŠMRLJ, Janez. N-(Propargyl)diazenecarboxamides for 'click' conjugation and their 1, 3-dipolar cycloadditions with azidoalkylamines in the presence of Cu(II). *Tetrahedron*. [Print ed.], 2010, vol. 66, no. 14, str. 2602–2613, doi: 10.1016/j.tet.2010.02.042. [COBISS.SI-ID 33776133]

OK15. KEPE, Vladimir, GHETTI, Bernardino, FARLOW, Martin R., BRESJANAC, Mara, MILLER, Karen, HUANG, Sung-Cheng, WONG, Koon-Pong, MURRELL, Jill Renee, PICCARDO, Pedro, EPPERSON, Francine, REPOVŠ, Grega, ŠMID, Lojze, PETRIČ, Andrej, SIDDARTH, Prabha, LIU, Jie, SATYAMURTHY, Nagichettiar, SMALL, Gary W., BARRIO, Jorge R. PET of brain prion amyloid in Gerstmann-Sträussler-Scheinker disease. *Brain pathol.*, 2010, vol. 20, no. 2, str. 419–430, doi: 10.1111/j.1750-3639.2009.00306.x. [COBISS.SI-ID 30622469]

OK16. URŠIČ, Uroš, SVETE, Jurij, STANOVNIK, Branko. Transformations of dimethyl (2E,3E)-2-[(dimethylamino) methylene]-3-(1-methyl-2, 5-dioxoimidazolidin-4-yl idene)succinate with C-nucleophiles. *Heterocycles*, 2010, vol. 82, no. 2, doi: 10.3987/COM-10-S(E)97. [COBISS.SI-ID 34691077]

OK17. WAGGER, Jernej, GROŠELJ, Uroš, Svete, Jurij, STANOVNIK, Branko. Synthesis of racemic, N-benzylated neoechinulin A and isoneoechinulin A. *Synlett*, no. 8, str. 1197–1200, doi: 10.1055/s-0029-1219812. [COBISS.SI-ID 33976069]

OK18. ŽEROVNIK, Darja, GROŠELJ, Uroš, KRALJ, David, MALAVAŠIČ, Črt, BEZENŠEK, Jure, DAHMANN, Georg, STARE, Katarina, MEDEN, Anton, STANOVNIK, Branko, Svete, Jurij. Synthesis of 1,5,6,7-tetrahydro-4H--pyrazolo[4,3-c]pyridin-4-ones as conformationally constrained pyrazole analogues of histamine. *Synthesis (Stuttg.)*, 2010, no. 19, str. 3363–3372, doi: 10.1055/s-0030-1257864. [COBISS.SI-ID 34495237]

OK19. BEZENŠEK, Jure, KOLEŠA, Tanja, GROŠELJ, Uroš, WAGGER, Jernej, STARE, Katarina, MEDEN, Anton, Svete, Jurij, STANOVNIK, Branko. [2+2] Cycloaddition of electron-poor acetylenes to (E)-3-dimethylamino-1--heteroaryl-prop-2-en-1-ones : synthesis of highly functionalized 1-heteroaroyl-1,3-butadienes. *Tetrahedron lett.*. [Print ed.], 2010, vol. 51, no. 26, str. 3392–3397, doi: 10.1016/j.tetlet.2010.04.106. [COBISS.SI-ID 34086917]

OK20. URŠIČ, Uroš, Svete, Jurij, STANOVNIK, Branko. Synthesis of 4-(2-hydroxy-1-methyl-5-oxo-1H-imidazol-4(5H)-ylidene)-5-oxo-1-aryl-4,5-dih ydro -1H-pyrrole-3-carboxylates, a new triazafulvalene system. *Tetrahedron*. [Print ed.], 2010, vol. 66, no. 24, str. 4346–4356, doi: 10.1016/j.tet.2010.04.025. [COBISS.SI-ID 34021893]

OK21. ŠIMUNEK, P., BAŠKOVČ, Jernej, GROŠELJ, Uroš, MEDEN, Anton, Svete, Jurij, STANOVNIK, Branko. The structure of the product formed by condensation of malononitrile with dialkyl acetone-1,3-dicarboxylates. *Z. Nat. forsch., B J. chem. sci.*, 2010, vol. 65b, no. 6, str. 807–810. [COBISS.SI-ID 34205957]

OK22. SVETE, Jurij, GROŠELJ, Uroš, BAŠKOVČ, Jernej, DAHMANN, Georg, STANOVNIK, Branko. Parallel solution-phase synthesis of (2S, 4E)-4-(arylaminomethylidene)pyroglutamic acids. *Z. Nat.forsch., B J. chem. sci.*, 2010, vol. 65b, no. 6, str. 811–820. [COBISS.SI-ID 34202373]

OK23. SEEBACH, Dieter, GROŠELJ, Uroš, SCHWEIZER, W. Bernd, GRIMME, Stefan, MÜCK-LICHTENFELD, Christian. Experimental and theoretical conformational analysis of 5-benzylimidazolidin-4-one derivatives : a 'playground' for studying dispersion interactions and a 'Windshield-Wiper' effect in organocatalysis. *Helv. Chim. Acta*, 2010, vol. 93, no. 1, str. 1–16, doi: 10.1002/hlca.200900376. [COBISS.SI-ID 33732101]

OK24. PETERLIN, Simona, PLANINŠEK, Odon, MOUTINHO, Isabel, FERREIRA, Paulo, DOLENC, Darko. Inverse gas chromatography analysis of spruce fibers with different lignin content. *Cellulose (Lond.)*, 2010, vol. 17, no. 6, str. 1095–1102, doi: 10.1007/s10570-010-9444-4. [COBISS.SI-ID 34565381]

OK25. TUTTLE, Tell, CERKOVNIK, Janez, KOLLER, Jože, PLESNIČAR, Božo. The search for protonated dihydrogen trioxide (HOOOH) : insights from theory and experiment. *J. phys. chem., A Mol. spectrosc. kinet. environ. gen. theory*, 2010, vol. 114, no. 30, str. 8003–8008, doi: 10.1021/jp103882e. [COBISS.SI-ID 34295813]

PREGLEDNI ZNANSTVENI ČLANEK / REVIEW ARTICLE

OK26. KRANJC, Krištof, KOČEVAR, Marijan. Microwave-assisted organic synthesis : general considerations and transformations of heterocyclic compounds. *Curr. org. chem.*, 2010, vol. 14, no. 10, str. 1050–1074, doi: 10.2174/138527210791130488. [COBISS.SI-ID 33971461]

OK27. STANOVNIK, Branko, GROŠELJ, Uroš. Dialkyl acetone-1,3-dicarboxylates and their mono- and bis(dimethylamino) methylidene derivatives in the synthesis of heterocyclic systems. *Adv. heterocycl. chem.*, 2010, vol. 100, str. 145–174, doi: 10.1016/S0065-2725(10)10005-1. [COBISS.SI-ID 33872645]

KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

OK28. KIMMEL, Roman, NEČAS, Marek, KAFKA, Stanislav, KOŠMRLJ, Janez, VÍCHA, Robert. 3-Ethyl-8-methoxy-4-(2,3,4,6-tetra-O-acetyl-ß-D-glucopyranosyloxy)quinolin- 2(1H)-one. *Acta crystallographica. E, Structure Reports*, 2010, vol. E66, no. 6, str. o1328–o1329 (11 str. suppl.), doi: 10.1107/S1600536810016636. [COBISS.SI-ID 34018565]

OK29. KASUNIČ, Marta, VERČEK, Bojan, MUŠIČ, Irena, GOLOBIČ, Amalija. 3-Benzamido-1-benzoyl-1H-pyrrol--2(5H)-one. *Acta crystallographica. E, Structure Reports*, 2010, vol. E66, no. 3, str. o687 (6 str. suppl.), doi: 10.1107/S1600536810006483. [COBISS.SI-ID 33745413]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

OK30. KOČEVAR, Marijan. Microwave-assisted catalyzed organic transformations : [plenary lecture]. V: 9th International Symposium of the Romanian Catalysis Society, June 23–26, 2010, Iasi, Romania. *Book of abstracts*. [S. l.: s. n.], 2010, str. 8–9. [COBISS.SI-ID 34178053]

OK31. POLANC, Slovenko. Various applications of nitrogen-containing molecules in organic synthesis : [plenary lecture]. V: 48th Meeting of the Serbian Chemical Society, Novi Sad, Serbia, April 17–18, 2010. *Program. i Kratki izvodi radova. Programme. & Book of Abstracts*. Beograd: Srpsko hemijsko društvo: Serbian Chemical Society, 2010, str. 4. [COBISS.SI-ID 33943301]

OK32. STANOVNIK, Branko. From [beta]-dimethylamino-[alpha]-acylamino-[alpha],[beta]-didehydro acid derivatives and related enaminones via heterocycles and heterocyclic amino acids to indole alkaloids : [plenary lecture]. V: KARTSEV, Viktor Georgievich (ur.). The Fourth International Conference CBC2010, August 2–6, 2010, Saint--Petersburg. *Sovremenye aspekty himii geterociklov : himija i biologičeskaja aktivnost sintetičeskih i prirodnyh soedinenij*. Moscow: ICSPF (International Charitable Scientific Partnership Foundation), 2010, str. 161–171. [COBISS.SI-ID 34321157]

OK33. GROŠELJ, Uroš. Strukture reaktivnih intermediatov pri organokatalizi z diarilprolinol etri in imidazolidinoni = Structures of reactive intermediates of organocatalysis with diarylprolinol ethers and imidazolidinones : [uvodno sekcijsko predavanje]. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–10. [COBISS.SI-ID 34446853]

OK34. ŠTEFANE, Bogdan. Reaktivnost in pretvorbe 1,3-dioksa-BF[spodaj]2 kelatov = Reactivity and transformations of 1,3-dioxa-BF[sub]2 chelates : [uvodno sekcijsko predavanje]. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–6. [COBISS.SI-ID 34452229]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

OK35. BAŠKOVČ, Jernej, Svete, Jurij, STANOVNIK, Branko. Razvoj metod za kombinatorno sintezo N-substituiranih 1,6-dihidropiridin-3-karboksamidov = Developement of methods for combinatorial synthesis of N-substituted 1,6-dihydropyridine-3-carboxamides. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–3. [COBISS.SI-ID 34454021]

OK36. BEZENŠEK, Jure, KOLEŠA, Tanja, GROŠELJ, Uroš, WAGGER, Jernej, STARE, Katarina, MEDEN, Anton, Svete, Jurij, STANOVNIK, Branko. [2+2] Cikloadicije elektronsko revnih acetilenov na »push-pull« dimetilaminopropenoate = [2+2] Cycloadditions of electron-poor acetylenes on push-pull dimethylaminopropenoates. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–7. [COBISS.SI-ID 34459397]

OK37. GAZVODA, Martin, KRANJC, Krištof, POLANC, Slovenko, KOČEVAR, Marijan. Sinteza izoindolov z Diels-Alderjevo reakcijo 2H-piran-2-onov ob prisotnosti dehidrogenacijskega katalizatorja = Synthesis of isoindoles by the Diels-Alder reaction of 2H-pyran-2-ones in the presence of dehydrogenation catalyst. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. [1–5]. [COBISS.SI-ID 34453765]

OK38. JURANOVIČ, Amadej, KRANJC, Krištof, POLANC, Slovenko, KOČEVAR, Marijan. Primerjalna študija reakcijskih poti Diels-Alderjeve reakcije na 2H-piran-2-onih pod vplivom mikrovalov in visokotlačnimi pogoji = Comparative study of reaction pathways of the Diels-Alder reaction on 2H-pyran-2-ones under microwave-assisted conditions and high pressures. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–7. [COBISS.SI-ID 34453253]

OK39. KOVAČ, Nives, GLAVAŠ, Neli, ŠKET, Boris. Petola-stromatolitic basement for manual gathering of salt in Secovlje salina. *Rapp. P-V. Réun. – Comm. Int. Explor. Sci. Mer Mediterr.*, 2010, vol. 39, št. 1, str. 270. [COBISS.SI-ID 2223951]

OK40. KRANJC, Krištof, PERDIH, Franc, KOČEVAR, Marijan. Vpliv velikosti obroča na ekso/endo selektivnost pri dvojni termični Diels-Alderjevi reakciji pripojenih piran-2-onov = Effects of ring size on the exo/endo selectivity of a thermal double Diels-Alder reaction of fused pyran-2-ones. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–8. [COBISS.SI-ID 34459141]

OK41. MALAVAŠIČ, Črt, WAGGER, Jernej, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, Svete, Jurij. Priprava, struktura in uporabnost kiralnih N-alkiliranih cikličnih dipeptidov = Preparation, structure and applicability of chiral N-alkylated cyclic dipeptides. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–9. [COBISS.SI-ID 34449413]

OK42. MOZER, Alenka, ČEPIČ, Mojca, DOLENC, Darko. Gimnazija Vič students' science projects in cooperation with research institutions. V: DOLINŠEK, Slavko (ur.). XIV. IOSTE Symposium, International Organization for Science and Technology Education, June 13.–18. 2010, Bled, Slovenia. *Socio-cultural and human values in science and technology education : proceedings*. Ljubljana: Institute for Innovation and Development of University, 2010, str. 1–8, ilustr. [COBISS.SI-ID 8348745]

OK43. POŽGAN, Franc. Rutenijevi kompleksi kot katalizatorji za direktno funkcionalizacijo sp[na]2-C-H vezi z aril halidi = Ruthenium complexes as catalysts for direct functionalisation of sp[sup]2-C-H bonds with aryl halides. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–6. [COBISS.SI-ID 34449669]

OK44. VRAŽIČ, Dejan, JEREB, Marjan, STAVBER, Stojan, LAALI, Kenneth K. Halogeniranje organskih spojin z NXS reagenti v ionskih tekočinah = Halogenation of organic compounds in ionic liquids using NXS reagents. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], 7 str. [COBISS.SI-ID 23964199]

OBJAVLJENI POVZETEK ZNANSTVENEGA PRISPEVKA NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION ABSTRACT (INVITED LECTURE)

OK45. GROŠELJ, Uroš. Insight into the structures of reactive intermediates of organocatalysis with diarylprolinol ethers and imidazolidinones : [invited lecture]. V: *24th European colloquium on heterocyclic chemistry : August 23rd – 27th, 2010*. Gumpoldskirchen: Book-of-Abstracts.com, 2010, str. IL–11. [COBISS.SI-ID 34400517]

OK46. DOLENC, Darko. Laser flash photolysis of organic iodine compounds. The formation of 9-I-2 iodanyl radicals : [invited lecture]. V: CHATGILIALOGLU, Chryssostomos (ur.). *Proceedings of EUCHEM Conference on Organic Free Radicals : June 28 – July 2, 2010, Bologna, Italy*. 1st ed. Roma: MMX Arachne, 2010, str. 58. [COBISS.SI-ID 34230021]

SREDNJEŠOLSKI, OSNOVNOŠOLSKI ALI DRUGI UČBENIK Z RECENZIJO / REVIEWED SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK

OK47. ČEH, Boris, DOLENC, Darko. *Snovi, okolje, prehrana : učbenik za kemijo v srednjih strokovnih šolah*. 1. izd. Ljubljana: DZS, 2010. 168 str., ilustr. ISBN 978-961-02-0077-2. [COBISS.SI-ID 252735232]

OK48. DOLENC, Darko, ŠKET, Boris. *Kemija za gimnazije 3, Učbenik za 3. letnik gimnazij*. 1. izd. Ljubljana: DZS, 2010. 192 str., ilustr. ISBN 978-961-02-0137-3. [COBISS.SI-ID 251647488]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

OK49. GLAŽAR, Saša A., GRAUNAR, Mojca, MODEC, Barbara, ŠKET, Barbara, ŠKET, Boris. *Kemija danes : učenje z nalogami : zbirka nalog za 8. in 9. razred devetletne osnovne šole*, (Raziskovalec 8), (Raziskovalec 9). 1. izd. Ljubljana: DZS, 2010. 184 str., ilustr. ISBN 978-86-341-3645-6. [COBISS.SI-ID 249326336]

OK50. DOLENC, Darko. *Vaje iz spektroskopije : tabele in spektroskopski problemi : gradivo za vaje iz organske analize : [interno študijsko gradivo]*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, 2010. 35 str., graf. prikazi. [COBISS.SI-ID 34341125]

PATENTNA PRIJAVA / PATENT APPLICATION

OK51. OSMAK, Maja, POLANC, Slovenko, ČIMBORA, Tamara, BROZOVIĆ, A., KOČEVAR, Marijan, MAJCE, Vita, ALIČ, Branko. *Analogues of 1, 3-bis(4-nitrophenyl)triazenes, their pharmaceutically acceptable salts and N-acyl derivatives for tumor treatment : patentna prijava : WO 2010103338 (A1), 2010-09-16*. [S. l.]: World Intellectual Property Organization, 2010. 21 str., ilustr. [COBISS.SI-ID 30639621]

OK52. TUREL, Iztok, KLJUN, Jakob, ŠTEFANE, Bogdan. *Postopek za pripravo racemnega nikotina : št. P-201000450*. Ljubljana: Urad Republike Slovenije za intelekturalno lastnino, 22.12.2010. 7 str. [COBISS.SI-ID 34764549]

OK53. KIDEMET, Davor, ZUPET, Rok, SMODIŠ, Janez, ŠTEFANE, Bogdan, POŽGAN, Franc. *Process and intermediates for the preparation of aliskiren : Application No. 09176568.5-1211*. Rijswijk: European Patent Office, 11. 1. 2010. [COBISS.SI-ID 33647109]

OK54. ČASAR, Zdenko, KOŠMRLJ, Janez. *Key intermediates for the synthesis of rosuvastatin or pharmaceutically acceptable salts thereof : international application no.: WO 2010/086438 A1*. [S. l.]: World Intellectual Property Organization, International Bureau, 5.08.2010. 40 str., graf. prikazi. [COBISS.SI-ID 34323205]

PATENT / PATENT

OK55. ANDERS, Manfred, LICHTBLAU, Dirk Andreas, KOLAR, Jana, MALEŠIČ, Jasna, STRLIČ, Matija, ŠALA, Martin, KOČEVAR, Marijan. *Antioxidant for an organic material and method for treating the same : patent : EP 1664431 (B1), 2010-08-04*. [S. l.]: European Patent Office, 2010. 21 str., ilustr. [COBISS.SI-ID 26939909]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

OK56. STANOVNIK, Branko. *New methodologies in organic synthesis: from heterocycles to natural products : [Kosova Academy of Sciences and Arts, Prishtina, 25. June, 2010]*. Prishtina, 2010. [COBISS.SI-ID 34177285]

UREDNIK / EDITORSHIP

OK57. *Acta chimica slovenica*. STANOVNIK, Branko (predsednik uredniškega sveta 1995–, član uredniškega odbora 1976–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]

OK58. *Acta chimica slovenica*. KRANJC, Krištof (član uredniškega sveta 2007–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]

OK59. *Acta chimica slovenica*. CERKOVNIK, Janez (urednik 2006–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]

OK60. *Advances in heterocyclic chemistry*. STANOVNIK, Branko (član uredniškega odbora 2003–). New York [etc.]: Academic Press, 1963–. ISSN 0065-2725. [COBISS.SI-ID 486917]

OK61. *ARKIVOC*. STANOVNIK, Branko (urednik 2010–, član uredniškega sveta 2010–). [Print ed.]. Gainesville: Arkat USA Inc., 2000–. ISSN 1424-6376. [COBISS.SI-ID 28057605]

OK62. *Croatica chemica acta*. STANOVNIK, Branko (član uredniškega odbora 1985–). Zagreb: Hrvatsko kemijsko društvo, 1956–. ISSN 0011-1643. [COBISS.SI-ID 22807]

OK63. *Journal of heterocyclic chemistry*. STANOVNIK, Branko (član uredniškega odbora 1997–). Provo, Utah, etc.: HeteroCorporation. ISSN 0022-152X. [COBISS.SI-ID 25749248]

OK64. *Molecules*. STANOVNIK, Branko (član uredniškega odbora 1998–). Berlin: Springer; Basel: Molecular Diversity Preservation International. ISSN 1420-3049. [COBISS.SI-ID 18462981]

OK65. *Targets in heterocyclic systems chemistry and properties*. STANOVNIK, Branko (član uredniškega odbora 2000–). Roma: Società Chimica Italiana. ISSN 1724-9449. [COBISS.SI-ID 1365807]

OK66. *Trends in Heterocyclic Chemistry*. STANOVNIK, Branko (član uredniškega odbora 2006–). Trivandrum: Research Trends. ISSN 0972-432X. [COBISS.SI-ID 1365551]

OK67. *Periodica polytechnica. Chemical engineering*. KOČEVAR, Marijan (član uredniškega odbora 2003–). Budapest: Technical University Budapest. ISSN 0324-5853. [COBISS.SI-ID 405018]

OK68. *Topics in heterocyclic chemistry*. POLANC, Slovenko (član uredniškega odbora 2008–). Heidelberg; Berlin: Springer. ISSN 1861-9282. [COBISS.SI-ID 33679621]

KATEDRA ZA ANORGANSKO KEMIJSKO TEHNOLOGIJO IN MATERIALE
CHAIR OF INORGANIC CHEMICAL TECHNOLOGY AND MATERIALS

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Jadran Maček

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Jadran Maček
prof. dr. Stane Pejovnik

v dopolnilnem razmerju / *part time*
prof. dr. Danilo Suvorov
izr. prof. dr. Miran Gaberšček
prof. dr. Venčeslav Kaučič

Asistenti / Assistants
mag. Barbara Novosel, viš. predavatelj
doc. dr. Klementina Zupan
doc. dr. Marjan Marinšek

Raziskovalec / Researcher
as. dr. Boštjan Genorio

Strokovni sodelavec / Research Assistant
dr. Vojmir Francetič

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Jana Kemperl	J. Maček	2006–2011	doktorski študij / *PhD*
Tina Skalar	J. Maček	2008–2013	doktorski študij / *PhD*
Tina Prinčič	S. Pejovnik	2009–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1.stopnje / *Bologna 1st Cycle Study Programmes*

Kemijsko inženirstvo / *Chemical Engineering* – UN:
Kemijska in procesna varnost / *Chemical and Process Safety*
Materiali za inženirje / *Engineering Materials*

Tehniška varnost / *Technical Safety* – UN:
Osnove materialov / *Fundamentals of Materials*
Nevarne snovi / *Hazardous Substances*

Kemijska tehnologija / *Chemical Technology* – VS:
Osnove industrijske kemije / *Fundamentals of Industrial Chemistry*
Procesi v industrijski kemiji / *Processes in Industrial Chemistry*
Mehanske operacije (izbirni predmet) / *Mechanical Operations (elective course)*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Gradiva / *Materials* – UN
Anorganski materiali in produkti, tehnična keramika in silikati / *Inorganic Materials and Products, Technical Ceramics and Silicates* – UN
Anorganski procesi in produkti / *Inorganic Processes and Products* – VS
Anorganska kemijska tehnologija / *Inorganic Chemical Technology* – UN
Pregled tehnologij / *Principles of Technological Processes* – UN
Nevarne snovi / *Hazardous Substances* – VS

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Materiali / *Materials*
Tehnična keramika in silikati / *Technical Ceramics and Silicates*
Kemijski procesi za sodobne materiale / *Chemical Processes for Advanced Materials*
Industrijske odpadne snovi / *Industrial Waste Materials*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1.stopnje / *Bologna 1st Cycle Study Programmes*

Tehnologija materialov I / *Technology of Materials I* ALUO – UN
Tehnologija materialov II / *Technology of Materials II* ALUO – UN
Industrijski materiali (izbirni predmet) / *Industrial Materials (elective course)* FMF – VS

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Keramika I / *Ceramics I* NTF – UN

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

- Raziskave in razvoj anorganskih materialov in produktov ter procesov za njihovo pripravo, materiali in kompoziti za visokotemperaturne gorivne celice, karakterizacija materialov / *Research and Development of Inorganic Materials, Products and Processes for their Preparation; Materials and Composites for High Temperature Fuel Cells; Characterization of Materials*
- Nanomateriali in nanokompoziti / *Nanomaterials and Nanocomposites*
- Industrijske odpadne snovi / *Industrial Waste Materials*
- Vpliv defektne strukture na sintranje oksidov, pretežno rutila / *Defect Structure Influence on Sintering of Oxides (Mostly Rutile)*
- Eksperimentalna verifikacija in statistična analiza veljavnosti različnih modelov procesa sintranja / *Experimetal Verification and Statistical Analysis of Different Sintering Models*
- Proučevanje procesa sintranja v prisotnosti tekoče faze ter sintranja v kemijsko heterogenih sistemih / *Study of Liquid Phase Sintering and Sintering in Heterogeneous Systems*
- Razvoj in uporaba impedančne spektroskopije za proučevanje ionskih prevodnikov in meje ionski prevodnik-kovina; znaten del aktivnosti poteka tudi na področju Li ionskih akumulatorjev / *Impedance Spectroscopy Method for the Development of Ionic Conductors and Ionic Conductor-Metal Boundary Characterisation*
- Sinteza in karakterizacija keramičnih in kompozitnih materialov za visokotemperaturne tehnologije npr. visokotemperaturne gorivne celice / *Synthesis and Characterisation of Ceramic and Composite Materials for High Temperature Technologies e.g. High Temperature Fuel Cells*
- Priprava kompleksnih keramičnih oksidov, mešanih oksidov in kompozitov z uporabo sol-gel tehnike in zgorevalne sinteze / *Sol-Gel and Combustion Synthesis Techniques for Complex Ceramic Oxides, Mixed Oxides and Preparation of Composites*
- Sinteza, karakterizacija in raziskave lastnosti enodimenzionalnih nanostrukturnih materialov / *Synthesis, Characterisation and Properties of One-Dimensional Nanostructured Materials*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- J. Moškon, Preglova nagrada Kemijskega inštituta za izjemna doktorska dela na področju kemije in sorodnih ved 2010 (mentor S. Pejovnik, somentor M. Gaberšček) / *Pregl Award of the National Institute of Chemistry 2010*
- M. Gaberšček, Preglova nagrada Kemijskega inštituta za izjemne dosežke na področju kemije in sorodnih ved 2010 / *Pregl Award of the National Institute of Chemistry 2010*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Netzsch STA 409 aparatura za simultano termično analizo / *Apparatus for Simultaneous Thermal Analysis*
- Mettler TA 4000:
  - TG 50 modul / *TG 50 Module*
  - DSC 20 modul / *DSC 20 Module*
- Masni spektrometer Pfeiffer / *Mass Spectrometer Pfeiffer*
- Agilent Micro GC 3000A, plinski kromatograf / *Gas Chromatograph*
- Vrstični elektronski mikroskop Jeol T300 / *Scanning Electron Microscope Jeol T300*
- Segrevalni mikroskop Leitz Wetzlar 301-200-301 / *Heating Microscope Leitz Wetzlar 301-200-301*
- Optični mikroskop za metalografske preiskave Leitz / *Optical Microscope Leitz*
- Analizator velikosti in porazdelitve velikosti delcev Fritzsch Analysette 22 / *Particle Sizer Fritzsch Analysette 22*
- Impedančni spektrometer / *Impedance Analyser*
- *1250 Frequency Response Analyser Solartron Schlumberg*
- *1286 Electrochemical Interface Solartron Schlumberg*
- Mikroskop na atomsko silo Nanoeducator NT-MTD / *Atomic Force Microscope Nanoeducator NT-MTD*
- Vrstični elektronski mikroskop na poljsko emisijo Zeiss ULTRA plus / *Field Emission Scanning Electron Microscope Zeiss ULTRA plus*
- Netzsch STA 449 F3 Jupiter aparatura za simultano termično analizo / *Netzsch STA 449 F3 Jupiter Apparatus for Simultaneous Thermal Analysis* (CO-NOT)
- Masni spektrometer Netzsch QMS 403C Aëolos / *Mass Spectrometer Netzsch QMS 403C Aëolos* (CO-NOT)
- Analizator specifične površine in poroznosti Micromeritics ASAP 2020 / *Surface Area and Porosity Analyzer Micromeritics ASAP 2020* (CO-NOT)

SODELOVANJE V CENTRIH ODLIČNOSTI / CENTERS OF EXCELLENCE

Center odličnosti: CO NOT – Nizkoogljične tehnologije / *Center of Excellence: Low-Carbon Technologies*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P–0175 Sinteza, struktura, lastnosti snovi in materialov / *Synthesis, Structure and Properties of Compounds and Materials*
Vodja programa / *Principal Researcher*: I. Leban

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L2–1157 Kompoziti za litijeve baterije z veliko močjo / *Composites for High Power Lithium Batteries*
Nosilec / *Principal Researcher*: R. Dominko (KI)
Sofinancer / *Co-sponsored by:* Iskra TELA

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

ATM1. LUKEŽIČ, Marjan, MARINŠEK, Marjan, FAGANELI, Jadran. Evaluation of burning test rate method for flammable solids to increase air-cargo safety. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 129–135. [COBISS.SI-ID 33808901]

ATM2. MARINŠEK, Marjan, ZUPAN, Klementina. Microstructure evaluation of sintered combustion-derived fine powder NiO-YSZ. *Ceram. int.*. [Print ed.], 2010, vol. 36, no. 3, str. 1075–1082. [COBISS.SI-ID 34080773]

ATM3. BITENC, Marko, PODBRŠČEK, Peter, DUBČEK, Pavo, BERNSTORFF, Sigrid, DRAŽIĆ, Goran, OREL, Bojan, PEJOVNIK, Stane, CRNJAK OREL, Zorica. In and ex situ studies of the formation of layered microspherical hydrozinciteas precursor for ZnO. *Chemistry (Weinh., Print)*. [Print ed.], 2010, vol.16, issue 37, str. 11481–11488. [COBISS.SI-ID 23869479]

ATM4. PODBRŠČEK, Peter, DRAŽIĆ, Goran, PARAMO, Jorge Antonio, STRZHEMECHNY, Yuri M., MAČEK, Jadran, CRNJAK OREL, Zorica. Growth of zinc oxide particles in the presence of silicon. *CrystEngComm (Camb., Online)*, 2010, vol.12, issue 10, str. 3071–3079. [COBISS.SI-ID 23749159]

ATM5. DOMINKO, Robert, VIDAL-ABARCA GARRIDO, Candela, BELE, Marjan, KÜZMA, Mirjana, ARČON, Iztok, GABERŠČEK, Miran. Electrochemical characteristics of Li[sub]2-x VTiO[sub]4 rock salt phase in Li-ion batteries. *J. power sources*. [Print ed.], 2010, [7] str., ilustr. [COBISS.SI-ID 4519962]

ATM6. ATEBAMBA, Jean-Marcel, MOŠKON, Jože, PEJOVNIK, Stane, GABERŠČEK, Miran. On the interpretation of measured impedance spectra of insertion cathodes for lithium-ion batteries. *J. Electrochem. Soc.*, 2010, vol. 157, no. 11, str. A1218–A1228, ilustr. [COBISS.SI-ID 4520474]

ATM7. DOMINKO, Robert, SIRISOPANAPORN, Chutchamon, MASQUELIER, Christian, HANŽEL, Darko, ARČON, Iztok, GABERŠČEK, Miran. On the origin of the electrochemical capacity of Li [sub] 2 Fe [sub] 0.8 Mn [sub] 0.2 SiO [sub] 4. *J. Electrochem. Soc.*, 2010, vol. 157, no. 12, str. A1309–A1316. [COBISS.SI-ID 1613051],

ATM8. GENORIO, Boštjan, STRMČNIK, Dušan, SUBBARAMAN, Ram, TRIPKOVIC, Dusan, KARAPETROV, Goran, STAMENKOVIC, Vojislav, PEJOVNIK, Stane, MARKOVIC, Nenad M. Selective catalysts for the hydrogen oxidation and oxygen reduction reactions by patterning of platinum with calix[4]arene molecules. *Nature materials*, 2010, vol. 9, no. 12, str. 998–1003. [COBISS.SI-ID 34569477]

ATM9. DREYER, Wolfgang, JAMNIK, Janko, GUHLKE, Clemens, HUTH, Robert, MOŠKON, Jože, GABERŠČEK, Miran. The thermodynamic origin of hysteresis in insertion batteries. *Nature materials*, 2010, vol. 9, str. 448–453. [COBISS.SI-ID 4476186]

KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

ATM10. GENORIO, Boštjan, PIRNAT, Klemen, CERC KOROŠEC, Romana, DOMINKO, Robert, GABERŠČEK, Miran. Electroactive organic molecules immobilized onto solid nanoparticles as a cathode material for lithium-ion batteries. *Angew. Chem. (Int. ed., Print)*. [Print ed.], 2010, vol. 49, no. 40, str. 7222–7224. [COBISS.SI-ID 34436869]

OBJAVLJENI POVZETEK ZNANSTVENEGA PRISPEVKA NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION ABSTRACT (INVITED LECTURE)

ATM11. ZUPAN, Klementina. Quantitative microstructural analysis : [invited lecture]. V: BENČAN, Andreja (ur.), KUŠČER, Danjela (ur.), MALIČ, Barbara (ur.), KOSEC, Marija (ur.). *Workshop on structural characterisation : Jožef Stefan Institute, Ljubljana, Slovenia, 28 January 2010 : [program and abstract book]*. Ljubljana: Institut Jožef Stefan, Electronic Ceramic Department, 2010, str. 9. [COBISS.SI-ID 34085637]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

ATM12. GOLOB, Janvit, LIKOZAR, Blaž, KOZLEVČAR, Bojan, FRANCETIČ, Vojmir, NOGRAŠEK, Boštjan, DEVETAK, Marko. *Razvoj tehnologij enkapsulacije gnojil : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 22 f., ilustr. [COBISS.SI-ID 34475269]

PATENT / PATENT

ATM13. UKMAR, Tina, GODEC, Aljaž, MAVER, Uroš, GENORIO, Boštjan, BELE, Marjan, PLANINŠEK, Odon, GABERŠČEK, Miran, JAMNIK, Janko. Sterično stabilizirana disperzija hibridnega anorgansko-organskega materiala v okolju kot pripravek za zaščito pred UV žarki ter postopek priprave : patent : SI 22859 (A), 2010-03-31. Ljubljana: Urad RS za intelektualno lastnino, 2010. 17 str., ilustr. [COBISS.SI-ID 4272666]

UREDNIK / EDITORSHIP

ATM14. *Acta chimica slovenica*. Kaučič, Venčeslav (član uredniškega odbora 1998–), Pejovnik, Stane (član uredniškega odbora 1998–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [COBISS.SI-ID 14086149]

ATM15. *International journal of molecular sciences*. Kaučič, Venčeslav (član uredniškega odbora 2001–). Basel: MDPI Center. ISSN 1422-0067. [COBISS.SI-ID 2779162]

ATM16. *Microporous and mesoporous materials*. Kaučič, Venčeslav (član uredniškega odbora 2003–). Amsterdam (etc.): Elsevier, 1998–. ISSN 1387-1811. [COBISS.SI-ID 1595162]

KATEDRA ZA KEMIJSKO, BIOKEMIJSKO IN EKOLOŠKO INŽENIRSTVO

CHAIR OF CHEMICAL, BIOCHEMICAL AND ENVIRONMENTAL ENGINEERING

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Aleksander Pavko

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
akademik prof. dr. Janez Levec
prof. dr. Aleksander Pavko
prof. dr. Marin Berovič
prof. dr. Igor Plazl
izr. prof. dr. Jana Zagorc Končan
doc. dr. Ana Lakota

Asistenti / Assistants
doc. dr. Andreja Zupančič Valant
doc. dr. Andreja Žgajnar Gotvajn
doc. dr. Polona Žnidaršič Plazl
doc. dr. Blaž Likozar

Tehniki / Technicians
Klemen Birtič
Vesna Delalut
Dušan Komel
Matija Matajdl, univ. dipl. inž.

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Andrej Pohar	I. Plazl	2007–2012	doktorski študij / *PhD*
Janja Babič	A. Pavko	2005–2010	doktorski študij / *PhD*
Mirjan Švagelj	M. Berovič	2006–2011	doktorski študij / *PhD*
Gorazd Stojkovič	P. Žnidaršič Plazl	2008–2013	doktorski študij / *PhD*
Matjaž Berlot	M. Berovič	2009–2013	doktorski študij / *PhD*
Uroš Novak	P. Žnidaršič Plazl	2010–2014	doktorski študij / *PhD*
Martin Lubej	I. Plazl	2010–2014	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemijsko inženirstvo / Chemical Engineering – UN:

Osnove okoljskega inženirstva (izbirni predmet) / *Introduction to Environmental Engineering (elective course)*

Tehniška varnost / *Technical Safety* – UN:

Varstvo okolja I / *Environmental Protection I*

Kemijska tehnologija / *Chemical Technology* – VS:

Osnove biokemije z biotehnologijo / *Fundamentals of Biochemistry with Biotechnology*

Biotehnološki procesi in naprave (izbirni predmet) / *Processes and Equipment in Biotechnology (elective course)*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Prenos toplote in snovi / *Heat and Mass Transfer* – UN

Osnove kemijske tehnike / *Fundamentals of Chemical Engineering* – VS

Načrtovanje procesov in ekološko inženirstvo / *Process Design and Environmental Engineering* – UN

Kemijsko reakcijsko inženirstvo / *Chemical Reaction Engineering* – UN

Osnove kemijske tehnike / *Fundamentals of Chemical Engineering* – UN

Biotehnologija / *Biotechnology* – UN

Pregled biokemijskih tehnologij / *Biotechnological Processes* – UN

Biokemijsko inženirstvo in biotehnologija / *Biochemical Engineering and Biotechnology* – UN

Biotehnologija z biokemijskim inženirstvom / *Biotechnology and Biochemical Engineering* – UN

Mehanske operacije / *Mechanical Operations* – VS

Kemijska inženirska kinetika / *Chemical Engineering Kinetics* – VS

Kemija okolja / *Environmental Chemistry* – UN

Ekološko inženirstvo / *Environmental Engineering* – UN

Industrijska ekologija in ekološko inženirstvo / *Industrial Ecology and Environmental Engineering* – VS

Kemijsko procesno računstvo / *Chemical Process Calculations* – UN

Modeliranje procesov / *Process Modelling* – UN

Načrtovanje procesov in naprav / *Process and Equipment Design* – VS

Kemijsko inženirski praktikum / *Chemical Engineering Practicals* – UN

Kemijsko inženirski praktikum / *Chemical Engineering Practicals* – VS

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Izbrana poglavja iz biotehnoloških procesov / *Advanced Bioprocess Engineering*

Izbrana poglavja iz transportnih pojavov / *Applied Transport Phenomena*

Izbrana poglavja iz okoljskega inženirstva / *Selected Topics in Environmental Engineering*

Izbrana poglavja iz kemijskega reakcijskega inženirstva / *Selected Topics in Chemical Reaction Engineering*

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Izbrana poglavja iz transportnih pojavov / *Applied Transport Phenomena*

Analiza in načrtovanje kemijskih reaktorjev / *Analysis and Design of Chemical Reactors*

Izbrana poglavja iz dinamike fluidov / *Dynamics of Fluids*

Izbrana poglavja iz biokemijskega inženirstva / *Selected Topics in Biochemical Engineering*

Površinske vode / *Surface Waters*

Ekotoksikologija / *Ecotoxicology*

IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemijske in fizikalne osnove / *Chemical and Physical Principles* – ALUO

Naravoslovje v restavratorstvu I, II, III / *Natural Sciences in Restoration I, II, III* – ALUO

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Procesna tehnika v živilstvu / *Food Technology* BF – UN

Zaključni procesi v biotehnologiji / *Downstream Processes in Biotechnology* BF – UN

Bolonjski programi 2. stopnje / *Bologna 2nd Cycle Master Study Study Programmes*

Industrijsko biokemijsko inženirstvo / *Industrial Biochemical Engineering* – BF

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Industrijska ekologija / *Industrial Ecology* – UL Interdisciplinarni doktorski študijski program Varstvo okolja / *UL Interdisciplinary Doctoral Study Programme in Environmental Protection*

Miniaturizacija naprav v bioprocesih / *Miniaturization in Bioprocessing* – UL Interdisciplinarni doktorski študijski program Bioznanosti / *UL Interdisciplinary Doctoral Study Programme in Biosciences*

Modeliranje bioprocesov / *Bioprocess Modelling* – UL Interdisciplinarni doktorski študijski program Bioznanosti / *UL Interdisciplinary Doctoral Study Programme in Biosciences*

Kemija in tehnologija okolja / *Environmental Chemistry and Technology* –

UL Interdisciplinarni doktorski študijski program Varstvo okolja / *UL Interdisciplinary Doctoral Study Programme in Environmental Protection*

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Izbrana poglavja iz kemijskih in fizikalnih metod v restavratorstvu / *Chemical and Physical Methods in Restoration – Selected Topics* – ALUO

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

1. Raziskave s področja procesnega inženirstva / *Process Engineering Research*
   - Raziskave in razvoj znanj za tehnološko in okoljsko optimizacijo procesov / *Optimization Research in the Field of Process and Environmental Technology*
   - Reologija in mešanje / *Rheology and Mixing*
   - Snovni prenos v koloni z mehurčki / *Mass Transfer in a Bubble Column*

2. Raziskave s področja biokemijskega inženirstva / *Research in the Field of Biochemical Engineering and Biotechnology*
   - Raziskave in razvoj biotransformacij in izolacije bioproduktov v mikrofluidnih sistemih / *Research and Development of Biotransformations and Downstream Processes within Microfluidic Systems*
   - Adsorpcija farmacevtskih učinkovin v koloni s polnilom / *Adsorption of Pharmaceutical Compounds in a Packed Bed Column*

3. Raziskave s področja okoljskega inženirstva / *Research in the Field of Environmental Engineering*
   - Bioremedijacija z glivami bele trohnobe / *Bioremediation with White Rot Fungi*
   - Čiščenje močno onesnaženih odpadnih vod z naprednimi oksidacijskimi postopki / *Advanced Oxidation Processes for Treatment of Heavily Polluted Wastewaters*
   - Spremljanje učinkovitosti čiščenja odpadnih vod z biotesti / *Evaluation of Wastewater Treatment Efficiency Using Biotests*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

– M. Linec, Prešernova nagrada FKKT za leto 2010 (mentor J. Levec) / *The Faculty Prešeren Award for 2010*
– A. Lakota, pohvala Študentskega sveta za pedagoško delo na smeri Kemijsko inženirstvo / *Students Award for the Quality of Teaching in Chemical Engineering Study Programme*

ČLANSTVO V AKADEMIJAH / MEMBERSHIP IN ACADEMIES

– J. Levec, redni član Slovenske akademije znanosti in umetnosti / *Full Member, Slovenian Academy of Sciences and Arts*
– M. Berovič, član / *Member, New York Academy of Science*

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

– I. Plazl, *Chemical and Biochemical Engineering Quarterly*
– A. Pavko, glavni urednik / *Editor-in-Chief, Acta Chimica Slovenica*
– A. Pavko, *Food Technology and Biotechnology*
– M. Berovič, *Associate Editor, Biotechnology Annual Review*
– M. Berovič, *Editor, Biochemical Engineering, New Biotechnology*
– J. Levec, *Acta Chimica Slovenica*
– J. Levec, *Chinese Journal of Chemical Engineering.*
– J. Levec, *International Journal of Chemical Engineering*
– J. Zagorc Končan, *European Water Management*
– P. Žnidaršič Plazl, *Chemical and Biochemical Engineering Quarterly*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

– Plinski kromatograf HP / *Gas Chromatograph HP*
– Tekočinski kromatograf Knauer / *HPLC Knauer*
– Tekočinski kromatograf Varian / *HPLC Varian*
– Rotacijski reometer HAAKE RS 150 / *Rheometer HAAKE RS 150*
– Rotacijski reometer HAAKE CV 20 / *Rheometer HAAKE CV 20*
– UV-VIS spektrofotometer Perkin Elmer Lambda 25 / *UV-VIS Spectrophotometer Perkin Elmer Lambda 25*
– Mikrovalovni reaktor / *Microwave Reactor*
– Laboratorijski bioreaktor / *Benchtop Fermenter Type KLF 2000*

- TOC 5000A Shimadzu aparatura / *TOC 5000A Analyser Shimadzu*
- Vary 50 Varian spektrofotometer / *Vary 50 Varian Spectrophotometer*
- Aparatura za določanje toksičnosti LUMIStox Dr. Lange / *Luminometer for Toxicity Tests LUMIStox Dr. Lange*
- Aparatura aerobni digester W11-A / *Aerobic Digester W/11-A*
- Rotacijski reometer- Physica MCR 301 / *Modular Compact Rheometer Physica MCR 301*
- Merilni sistem Protos 3400C za merjenje raztopljenega kisika / *Measuring System Protos 3400C with DO Measuring Module*
- Laboratorijski bioreaktorji Bioengineering AG, 2, 5,10, 15 l / *Laboratory Bioreactors Bioengineering AG, 2, 5,10, 15 l*
- Laboratorijski bioreaktorji Chemap AG, 3x10 l / *Laboratory Bioreactors Chemap AG, 3x10 l*
- Stresalnik KS 40001 inkubatorski Control IKA/ *Thermostated Shaker Control IKA*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P2–0191 Kemijsko inženirstvo / *Chemical Engineering*
Vodja programa / *Principal Researcher*: M. Krajnc

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L4–2024 Vpliv tehnoloških postopkov na ohranjanje aromatskega potenciala v tehnologiji pridelave vin / *Influence of Process Technology on Aromatic Potential in Wine Fermentation*
Nosilec / *Principal Researcher*: M. Berovič
Sofinancer / *Co-sponsored by*: Perutnina Ptuj

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

Aplikativne raziskave na področju adsorpcije / *Applied Research in the Field of Adsorption*
Nosilec / *Principal Researcher*: A. Pavko
Financer / *Sponsored by*: Lek d.d., Ljubljana.

2/MK/2008 Razvoj novega materiala za jedro panela iz ekspandiranega perlita – faza V / *Development of New Material for Panel Core from Expanded Perlite – V*
Nosilec / *Principal Researcher*: I. Plazl
Financer / *Sponsored by*: Trimo Trebnje d.d., Trebnje

MEDNARODNO SODELOVANJE NA PODROČJU IZOBRAŽEVANJA / INTERNATIONAL COOPERATION IN THE FIELD OF EDUCATION

– A. Žgajnar Gotvajn, ERASMUS TEACHING EXCHANGE, Brno University of Technology, Faculty of Chemistry, Brno, Czech Republic.
– A. Žgajnar Gotvajn, ERASMUS TEACHING EXCHANGE, Norwegian University of Science and Technology (NTNU), Trondheim, Norway.
– A. Žgajnar Gotvajn, mentorica slovenske srednješolske ekipe na 3. mednarodni projektni olimpijadi raziskovalnih nalog s področja trajnostnega razvoja: energija, inženirstvo in okolje v Houstonu, ZDA, 2010 / *Mentor of the Slovenian Team at I-SWEEEP 2010 – the International Sustainable World Project Olympiad (Energy, Engineering & Environment), Houston, USA, 2010*

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Kitajska *Slovenia – China*	Produkcija farmacevtsko aktivnih spojin *Grifola frondoza* s postopkom gojenja na trdnem in tekočem gojišču / *Production of Pharmaceutically Active Compounds from Grifola Frondosa by Solid State and Submerged Cultivation* Nosilec / *Principal Researcher*: M. Berovič
Slovenija – Bolgarija *Slovenia – Bulgaria*	Mikrobiološke transformacije steroidov v sistemu mikrokanalov / *Microbial Transformations of Steroids within a Microchannel System* Nosilka / *Principal Researcher*: P. Žnidaršič Plazl
Slovenija – Portugalska *Slovenia – Portugal*	Implementacija mikrostrukturiranih naprav v procese biotransformacij in bioseparacij / *Implementation of Microstructured Devices in Biotransformation and Bioseparation Processes* Nosilec / *Principal Researcher*: I. Plazl

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

Mednarodno znanstveno sodelovanje, ki ga financira Nacionalna fundacija za znanost, visoko šolstvo in tehnološki razvoj Republike Hrvaške – raziskovalni projekt: Sinteza ionskih tekočin in biotransformacije s temi topili v mikroreaktorjih / *International Scientific Cooperation, sponsored by the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia – Research Project: Synthesis of Ionic Liquids and Biotransformations with these Solvents in Microreactors*
Nosilka / *Principal Researcher*: P. Žnidaršič Plazl

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK /ORIGINAL SCIENTIFIC ARTICLE

KIŽ1. LEVSTEK, Meta, PLAZL, Igor, ROUSE, Joseph D. Estimation of the specific surface area for a porous carrier. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 45–51. [COBISS.SI-ID 33804037]

KIŽ2. NAKRST, Jana, BISTAN, Mirjana, TIŠLER, Tatjana, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. Feasibility of Fenton's oxidation for removal of estrogens from aqueous solutions. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 90–99. [COBISS.SI-ID 33808389]

KIŽ3. PLAZL, Igor, LAKNER, Mitja. Modeling and finite difference numerical analysis of reaction-diffusion dynamics in a microreactor. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 100–109. [COBISS.SI-ID 33804805]

KIŽ4. TIŠMA, Marina, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor, VASIĆ-RAČKI, Đurđa, ZELIĆ, Bruno. Oxidation of coniferyl alcohol catalyzed by laccases from Trametes versicolor. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 110–117. [COBISS.SI-ID 33807109]

KIŽ5. TISU, Matjaž, PAVKO, Aleksander. Oxygen transfer in a laboratory stirred tank bioreactor during mammalian cell culture cultivation. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 123–128. [COBISS.SI-ID 33794309]

KIŽ6. STOJKOVIČ, Gorazd, ŽNIDARŠIČ PLAZL, Polona. Immobilization of yeast cells within microchannels of different materials. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 144–149. [COBISS.SI-ID 33807877]

KIŽ7. MERWE, Jacob D. van der, MINARIK, Martin, BEROVIČ, Marin, HERAKOVIČ, Niko. Heat transfer in citric acid production with axial and radial flow impellers. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 150–156. [COBISS.SI-ID 33809925]

KIŽ8. LIKOZAR, Blaž, MAJOR, Zoltan. Morphology, mechanical, cross-linking, thermal, and tribological properties of nitrile and hydrogenated nitrile rubber/multi-walled carbon nanotubes composites prepared by melt compounding : the effect of acrylonitrile content and hydrogenation. *Appl. surf. sci.*. [Print ed.], 2010, vol. 257, no. 2, str. 565–273. [COBISS.SI-ID 34274821]

KIŽ9. KLOFUTAR, Boštjan, GOLOB, Janvit, LIKOZAR, Blaž, KLOFUTAR, Cveto, ŽAGAR, Ema, POLJANŠEK, Ida. The transesterification of rapeseed and waste sunflower oils : mass-transfer and kinetics in a laboratory batch reactor and in an industrial-scale reactor/separator setup. *Bioresour. technol.*. [Print ed.], 2010, vol. 101, no. 10, str. 3333–3344. [COBISS.SI-ID 33677317]

KIŽ10. ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Development of a continuous steroid biotransformation process and product extraction within microchannel system. *Catal. today*. [Print ed.], 2010, vol. 157, no. 1/4, str. 315–320. [COBISS.SI-ID 33681925]

KIŽ11. MARQUES, M. P. C., FERNANDES, P., CABRAL, Joaquim M. S., ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. On the feasibility of in-situ steroid biotransformation and product recovery in microchannels. *Chem. eng. j. 1996*. [Print ed.], 2010, vol. 160, no. 2, str. 708–714. [COBISS.SI-ID 33911813]

KIŽ12. DERCO, Ján, ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana, ALMÁSIOVÁ, Beáta, KASSAI, Angelika. Pretreatment of landfill leachate by chemical oxidation processes. *Chem. zvesti*, 2010, vol. 64, no. 2, str. 237–245. [COBISS.SI-ID 33642501]

KIŽ13. BEESTON, Michael Philip, POHAR, Andrej, ELTEREN, Johannes Teun van, PLAZL, Igor, ŠLEJKOVEC, Zdenka, VEBER, Marjan, GLASS, Hylke J. Assessment of physical leaching processes of some elements in soil upon ingestion by continuous leaching and modeling. *Environ. sci. technol.*. [Print ed.], 2010, vol. 44, issue 16, str. 6242–6248. [COBISS.SI-ID 4448538]

KIŽ14. KOGEJ, Adela, LIKOZAR, Blaž, PAVKO, Aleksander. Lead biosorption by self-immobilized Rhizopus nigricans pellets in a laboratory scale packed bed column : mathematical model and experiment. *Food technol. biotechnol.*, 2010, vol. 48, no. 3, str. 344–351. [COBISS.SI-ID 34326021]

KIŽ15. LUKAČ, Bojana, ZUPANČIČ-VALANT, Andreja. Raziskovanje obnašanja gumibitumna kot veziva za proizvodnjo gumiranih asfaltnih zmesi = The investigation of rubber modified bitumen as a binder for production of asphalt mixtures. *Gradb. vestn.*, 2010, letn. 59, št. [10], str. 261–268. [COBISS.SI-ID 34588933]

KIŽ16. COTMAN, Magda, ŽGAJNAR GOTVAJN, Andreja. Comparison of different physico-chemical methods for the removal of toxicants from landfill leachate. *J. hazard. mater.*. [Print ed.], 2010, vol. 178, no. 1/3, str. 298–305. [COBISS.SI-ID 33885701]

KIŽ17. STOJKOVIČ, Gorazd, PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. L-Malic acid production within a microreactor with surface immobilised fumarase. *Microfluid. nanofluid. (Print)*, 2011, vol. 10, no. 3, str. 627–635. [COBISS.SI-ID 34517509]

KIŽ18. LIKOZAR, Blaž. Kinetic modeling of the peroxide cross-linking of polymer/monomer blends : from a theoretical model framework to its application for a complex polymer/monomer dispersion system. *React. funct. polym.*. [Print ed.]. [COBISS.SI-ID 34593029]

KIŽ19. LIKOZAR, Blaž. Diffusion of ionic liquids into elastomer/carbon nanotubes composites and tensile mechanical properties of resulting materials. *Sci. iran.*, 2010, vol. 17, no. 1, str. 35–42. [COBISS.SI-ID 34622213]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

KIŽ20. POHAR, Andrej, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Integrated process of transesterification within a microchannel system. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–4]. [COBISS.SI-ID 34497797]

KIŽ21. STOJKOVIČ, Gorazd, ŽNIDARŠIČ PLAZL, Polona. Whole-cell biocatalysis within microchannels. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–4]. [COBISS.SI-ID 34497029]

KIŽ22. TIŠMA, Marina, ZELIĆ, Bruno, VASIĆ-RAČKI, Đurđa, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Biocatalyzed oxidation of phenolic compounds in a microreactor. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–5]. [COBISS.SI-ID 34496261]

KIŽ23. PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. Reaction-diffusion dynamics in microreactors : modelling and experiments. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–5]. [COBISS.SI-ID 34497541]

KIŽ24. MARQUES, M. P. C., FERNANDES, P., CABRAL, Joaquim M. S., ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Steroid biotransformation and in situ separation within microchannel system. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–5]. [COBISS.SI-ID 34496517]

KIŽ25. CVJETKO, M., VORKAPIĆ-FURAČ, Jasna, POHAR, Andrej, ŽNIDARŠIČ PLAZL, Polona. Synthesis of ionic liquids and their use as solvents for biocatalysis in microreactors. V: ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010. *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010, str. [1–5]. [COBISS.SI-ID 34496773]

KIŽ26. ŠVAGELJ, Mirjan, BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Submerged and solid state cultivation of antitumor extra and intracellular fungai polysaccharides of Ganoderma lucidum and Grifola frondosa : [plenary lecture]. V: 5th International Bioengineering Congress, Izmir Turkey, June 16–19, 2010, Tepekule Convention Center. *Programme & abstracts*. [S. l.: s. n.], 2010, str. 4–9. [COBISS.SI-ID 34177029]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

KIŽ27. BERLOT, Matjaž, BEROVIČ, Marin. Decreasing of production of ethanol by Saccharomyces cerevisiae metabolism control : [lecture]. V: *33rd World Congress of Vine and Wine [and] 9th General Assembly of the OIV : 20–25 June 2010, Tbilisi, Georgia*. [S. l.: s. n.], 2010, str. [1–8]. [COBISS.SI-ID 34446597]

KIŽ28. LIKOZAR, Blaž. Comparison of adsorption equilibrium and kinetic models for a case study of vancomycin adsorption from fermentation broths. V: LIKOZAR, Blaž (ur.). EFB Bioprocess Engineering Master Course. *Abstracts*. [S. l.: s. n.], 2010, str. [1–5]. [COBISS.SI-ID 34493445]

KIŽ29. LIKOZAR, Blaž. Modelling of thermal degradation of microalgae Chlorella vulgaris and comparison of lipid extraction techniques from microalgae biomass. V: LIKOZAR, Blaž (ur.). EFB Bioprocess Engineering Master Course. *Abstracts*. [S. l.: s. n.], 2010, str. [1–5]. [COBISS.SI-ID 34493701]

KIŽ30. BERLOT, Matjaž, BEROVIČ, Marin. Increasing of production of glycerol by Saccharomyces cerevisiae metabolism control. V: LIKOZAR, Blaž (ur.). EFB Bioprocess Engineering Master Course. *Abstracts*. [S. l.: s. n.], 2010, str. [1–6]. [COBISS.SI-ID 34493189]

KIŽ31. ŽGAJNAR GOTVAJN, Andreja, KALČÍKOVÁ, Gabriela, ZUPANČIČ, Marija, ZAGORC-KONČAN, Jana. Determination of inhibitory effects of landfill leachate on nitrification. V: *Book of Abstracts of the Second International Symposium on Green Chemistry for Environment and Health : Mykonos, Royal Mykonian Hotel & Thalasso Spa, September 26–29, 2010 : Elektronski vir*. Thessaloniki: Grafima, 2010, str. [1–6]. [COBISS.SI-ID 34505477]

KIŽ32. ZAGORC-KONČAN, Jana, KALČÍKOVÁ, Gabriela, ŽNIDARŠIČ PLAZL, Polona, ŽGAJNAR GOTVAJN, Andreja. Is ionic liquid 1-butyl-3-methylpyridinium dicyanamide a green solvent?. V: *Book of Abstracts of the Second International Symposium on Green Chemistry for Environment and Health : Mykonos, Royal Mykonian Hotel & Thalasso Spa, September 26–29, 2010 : Elektronski vir*. Thessaloniki: Grafima, 2010, str. [1–6]. [COBISS.SI-ID 34504709]

KIŽ33. STOJKOVIČ, Gorazd, PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. L-Malic acid production within a microreactor : [lecture]. V: *CHISA 2010 : CD-ROM of full texts*. Praha: Czech Society of Chemical Engineering, 2010, str. [1–4]. [COBISS.SI-ID 34495493]

KIŽ34. ŽGAJNAR GOTVAJN, Andreja, NAKRST, Jana, BISTAN, Mirjana, TIŠLER, Tatjana, ZAGORC-KONČAN, Jana. Does oxidative treatment really degrade estrogens?. V: Protection and Restoration of the Environment X, 5–9 July 2010, Corfu, Greece. *Conference proceedings : Pre10*. [S. l.: s. n.], 2010, str. [1–8]. [COBISS.SI-ID 34232581]

KIŽ35. ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. Reduction of environmental impact of municipal landfill: oxidative treatment of biologically treated leachate. V: Protection and Restoration of the Environment X, 5–9 July 2010, Corfu, Greece. *Conference proceedings : Pre10*. [S. l.: s. n.], 2010, str. [1–8]. [COBISS.SI-ID 34232069]

KIŽ36. COTMAN, Magda, ŽGAJNAR GOTVAJN, Andreja. Physico-chemical treatments of landfill leachate for improvement operation of SBR. V: GIDARAKOS, Evangelos (ur.). *CRETE 2010 : executive summaries : 2nd International conference on Hazardous and industrial waste management, 5–8 October, Chania, Crete, Greece*. Chania: Technical University of Crete, 2010, 8 str. [COBISS.SI-ID 4537370]

KIŽ37. LIKOZAR, Blaž. The effect of nanotubes' content and their hydroxy- and carboxy-functionalization in (hydrogenated) nitrile rubber/(un)functionalized multi-walled carbon nanotubes composites prepared by melt compounding and their morphology, mechanical, structural, thermodynamic, and functional properties : [oral]. V: 3rd Conference on Nanostructures, March 10–12, 2010, Sharif University of Technology, International Campus, Kish Island, I. R. Iran. *Proceedings : NS 2010*. [S. l.: s. n.], 2010, str. [1–4]. [COBISS.SI-ID 33830149]

KIŽ38. LIKOZAR, Blaž. Morphology, mechanical, structural, and thermal properties of hydrogenated nitrile rubber/hydroxy-functionalized multi-walled carbon nanotubes/ionic liquid composites : the effect of ionic liquid content. V: 3rd Conference on Nanostructures, March 10–12, 2010, Sharif University of Technology, International Campus, Kish Island, I. R. Iran. *Proceedings : NS 2010*. [S. l.: s. n.], 2010, str. [1–4]. [COBISS.SI-ID 33830661]

KIŽ39. LIKOZAR, Blaž. Morphology, mechanical, structural, and thermal properties of hydrogenated nitrile rubber/hydroxy-functionalized multi-walled carbon nanotubes/ionic liquid composites : the effect of ionic liquid type. V: 3rd Conference on Nanostructures, March 10–12, 2010, Sharif University of Technology, International Campus, Kish Island, I. R. Iran. *Proceedings : NS 2010*. [S. l.: s. n.], 2010, str. [1–5]. [COBISS.SI-ID 33830405]

KIŽ40. ŽGAJNAR GOTVAJN, Andreja, KALČÍKOVÁ, Gabriela, ZAGORC-KONČAN, Jana. Assessment of biotreatability of mature municipal landfill leachate. V: *The proceedings of the 4th annual international experts´ conference : Enviro-mamagement 2010 : 12–14. October, 2010, Hotel Patria, Štrbské Pleso, Slovakia : landfills in Europe & waste mamagement*. Žilina: NMC spol. s r.o., 2010, str. [1–6]. [COBISS.SI-ID 34533637]

KIŽ41. KALČÍKOVÁ, Gabriela, VÁVROVÁ, Milada, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. Seasonal variations in municipal landfill leachate quality. V: *The proceedings of the 4th annual international experts´ conference : Enviro-mamagement 2010 : 12.–14. October, 2010, Hotel Patria, Štrbské Pleso, Slovakia : landfills in Europe & waste mamagement*. Žilina: NMC spol. s r.o., 2010, str. [1–7]. [COBISS.SI-ID 34533381]

KIŽ42. PAVKO, Aleksander. Acta Chimica Slovenica – slovenska znanstvena revija z največjim faktorjem vpliva. V: ZEMLJIČ, Igor (ur.), BOŽIČ, Maja (ur.). *Prost dostop do dosežkov slovenskih znanstvenikov : zbornik prispevkov 4. skupnega posvetovanja Sekcije za specialne knjižnice in Sekcije za visokošolske knjižnice Zveze bibliotekarskih društev Slovenije : proceedings of 4th Joint Conference of the Special Libraries Section and the Academic Libraries Section of the Slovenian Library Association, [Ljubljana, 27. in 28. oktober 2010]*. Ljubljana: Zveza bibliotekarskih društev Slovenije, 2010, str. 39–45. [COBISS.SI-ID 34555909]

KIŽ43. DJINOVIĆ, Petar, BATISTA, Jurka, LEVEC, Janez, PINTAR, Albin. Synthesis of ordered nanostructured CuO-CeO [sub] 2 catalysts by hard template method. V: GAIGNEAUX, E. M. (ur.). *Scientific bases for the preparation of heterogeneous catalysts : proceedings of the 10th international symposium, Louvain-la-Neuve, Belgium, July 11–15, 2010*, (Studies in surface science and catalysis, vol. 175). Amsterdam [etc.]: Elsevier, 2010, str. 245–248. [COBISS.SI-ID 4459546]

KIŽ44. TROŠT, Nina, PAVKO, Aleksander. Produkcija ligninolitičnih encimov z glivo Dichomitus squalens imobilizirano na bukovem lesu = Ligninolytic enzyme production by Dichomitus squalens immobilized on beech wood. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–4. [COBISS.SI-ID 34465541]

KIŽ45. BERCE, Peter, GOLOB, Janvit, LIKOZAR, Blaž. Rast mikroalge Chlorella vulgaris pod različnimi svetlobnimi režimi = Growth of microalgae Chlorella vulgaris under different exposures to light. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–6. [COBISS.SI-ID 34476805]

KIŽ46. KALČÍKOVÁ, Gabriela, VÁVROVÁ, Milada, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. Unconventional assessment of efficiency of wastewater treatment plant by phytotoxicity tests = Nekonvencionalen pristop k ocenjevanju učinkovitosti čistilne naprave s testi fitotoksičnosti. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–6. [COBISS.SI-ID 34460677]

KIŽ47. PIVAR, Robert, GOLOB, Janvit, LIKOZAR, Blaž. Analiza tehnoloških procesov od parnega reforminga do proizvodnje formaldehida = Analysis of technological processes from steam reforming to formaldehyde production. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–8. [COBISS.SI-ID 34476293]

KIŽ48. LAKOTA, Ana. Dvoparametrski celični model kolone z mehurčki = Two-parameters cell model of bubble column. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–8. [COBISS.SI-ID 34469893]

KIŽ49. PINTAR, Albin, BATISTA, Jurka, LEVEC, Janez. Katalizatorji na osnovi ogljikovih nanocevk v procesih čiščenja odpadnih vod = Carbon nanotube-based catalysts in water purification processes. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–9. [COBISS.SI-ID 34462469]

KIŽ50. SENICA, David, BURJA, Roman, DUNJKO, Leon, PAVKO, Aleksander. Koncentriranje aktivne farmacevtske učinkovine v organskem topilu: nanofiltracija ali uparjanje? = Concentration of active pharmaceutical ingredient in organic solvent: nanofiltration or evaporation?. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–9. [COBISS.SI-ID 34448901]

KIŽ51. LAPORNIK, Domen, GOLOB, Janvit, LIKOZAR, Blaž. Ravnotežje in prenos snovi pri sušenju agarnih gelov za pripravo rodenticida = Equilibrium and mass transfer during drying of agar gels for rodenticide preparation. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–10. [COBISS.SI-ID 34471173]

KIŽ52. KAVŠEK, Miha, GOLOB, Janvit, LIKOZAR, Blaž. Mikroenkapsulacija insekticida s polisečnino = Microencapsulation of insecticide with polyurea. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–11. [COBISS.SI-ID 34476549]

KIŽ53. NOGRAŠEK, Boštjan, KOZLEVČAR, Bojan, GOLOB, Janvit, LIKOZAR, Blaž. Načrtovanje integriranega procesa oplaščanja zrn umetnih gnojil in sušenja v fluidiziranem sloju = Design of integrated process of synthetic fertilizer coating process and drying in fluidized bed. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–11. [COBISS.SI-ID 34477061]

KIŽ54. PIVEC, Aleksandra, LAH, Branko, ŠVAGELJ, Mirjan, KLINAR, Dušan, BEROVIČ, Marin, BELŠAK, Nataša. Anaerobna digestija lignocelulozne biomase – predhodna obdelava substrata = Anaerobic digestion of lignocellulosic biomass – pretreatment. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–12. [COBISS.SI-ID 34462725]

KIŽ55. KALČÍKOVÁ, Gabriela, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. Comparison of different treatment approaches for landfill leachate. V: LORBER, Karl Erich (ur.). *Tagungsband zur 10. DepoTech Konferenz, Montanuniversität Leoben/Österrich, 3.– November 2010 : DepoTech 2010 : Abfallwirtschaft : Abfalltechnik : Deponietechnik und Altlasten*. Leoben: Montanuniversität Leoben: Institut für Nachhaltige Abfallwirtschaft und Entsorgungstechnik (IAE), 2010, str. 791–794. [COBISS.SI-ID 34574341]

KIŽ56. LUKAČ, Bojana, ZUPANČIČ-VALANT, Andreja. Raziskovanje obnašanja gumibitumna kot veziva za proizvodnjo gumiranih asfaltnih zmesi. V: 10. slovenski kongres o cestah in prometu, Portorož, 20.–22. oktober 2010. *Zbornik referatov*. Ljubljana: DRC – Družba za raziskave v cestni in prometni stroki Slovenije, 2010, str. 1294–1304. [COBISS.SI-ID 34598917]

KIŽ57. KALČÍKOVÁ, Gabriela, VÁVROVÁ, Milada, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. Application of physico-chemical methods for post-treatment of municipal landfill leachate. V: OMELKA, Ladislav (ur.), WEITER, Martin (ur.), DZIK, Petr (ur.). Studentská Odborná Konference Chemie a Společnost, Vysoké učení technické v Brně, Fakulta chemická, 3. prosince 2010. *Sborník přispěvků*. Brno: Vysoké učení technické v Brně, Fakulta chemická, 2010, str. [1–4]. [COBISS.SI-ID 34668805]

OBJAVLJENI POVZETEK ZNANSTVENEGA PRISPEVKA NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION ABSTRACT (INVITED LECTURE)

KIŽ58. ŽNIDARŠIČ PLAZL, Polona. Implementation of microstructured devices in biotransformation processes : [invited lecture]. V: JUNKAR, Mihael (ur.), VALENTINČIČ, Joško (ur.), SABOTIN, Izidor (ur.). *Microreactor Technology for Healthcare Applications, Fiesa, Slovenia, September 26th–28th 2010 : book of abstract of the ESF exploratory workshop*. Ljubljana: Laboratory for Alternative Technologies, Faculty of Mechanical Engineering, 2010, str. 14. [COBISS.SI-ID 34573061]

SAMOSTOJNI ZNANSTVENI SESTAVEK ALI POGLAVJE V MONOGRAFSKI PUBLIKACIJI / INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

KIŽ59. MITCHELL, David, BEROVIČ, Marin. Solid state bioprocessing. V: BEROVIČ, Marin (ur.), ENFORS, Sven-Olof (ur.). *Comprehensive bioprocess engineering : doctoral/post-doctoral*. Ljubljana: University, 2010, str. 209–238. [COBISS.SI-ID 34486277]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

KIŽ60. LIKOZAR, Blaž. *Osnove kemijske tehnike : Elektronski vir : interno študijsko gradivo za študente 3. letnika univeritetnega študijskega programa Kemija*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za kemijsko, biokemijsko in ekološko inženirstvo, 2010. 1 el. optični disk (418 str.), ilustr. [COBISS.SI-ID 34148357]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

KIŽ61. GOLOB, Janvit, LIKOZAR, Blaž, PIVAR, Robert, BENCIK, Dejan, PEČELIN, Peter. *Analiza tehnološkega procesa proizvodnje formaldehida po metaloksidnem postopku : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 24 f., ilustr. [COBISS.SI-ID 34520837]

KIŽ62. PAVKO, Aleksander, LIKOZAR, Blaž, SENICA, David. *Aplikativne raziskave na področju adsorpcije : ravnotežje in kinetika adsorpcije vankomicina na izbranem nosilcu v mešalnem reaktorju in koloni : prvo medfazno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za kemijsko, biokemijsko in ekološko inženirstvo, 2010. [24] f., ilustr. [COBISS.SI-ID 34399493]

KIŽ63. GOLOB, Janvit, LIKOZAR, Blaž, KOZLEVČAR, Bojan, FRANCETIČ, Vojmir, NOGRAŠEK, Boštjan, DEVETAK, Marko. *Razvoj tehnologij enkapsulacije gnojil : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 22 f., ilustr. [COBISS.SI-ID 34475269]

KIŽ64. GOLOB, Janvit, LIKOZAR, Blaž, KAVŠEK, Miha, MATJAŠIČ, Aleš, DEVETAK, Marko. *Razvoj tehnologij mikroenkapsulacije pesticidov : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 29 f., ilustr. [COBISS.SI-ID 34448645]

KIŽ65. GOLOB, Janvit, LIKOZAR, Blaž, LAPORNIK, Domen, DEVETAK, Marko. *Razvoj tehnologij rodenticidov : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 28 f., ilustr. [COBISS.SI-ID 34467077]

KIŽ66. ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana. Študija možnosti uporabe oksidacijskih postopkov predčiščenja in dodatnega čiščenja deponijskih izcednih vod deponije Unično : (interno delovno poročilo). Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za kemijsko, biokemijsko in ekološko inženirstvo, 2010. 18 f., ilustr. [COBISS.SI-ID 33752581]

PATENTNA PRIJAVA / PATENT APPLICATION

KIŽ67. BEROVIČ, Marin, MAKOVEC, Darko, BOŠKOVIĆ, Suzana. *Postopek magnetnega izločanja kvasne biomase iz penečega vina : patentna prijava št. P-201000434*. Ljubljana: Urad RS za intelektualno lastnino, 13. dec. 2010. [COBISS.SI-ID 24285223]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

KIŽ68. ŽGAJNAR GOTVAJN, Andreja. *Environmental problems in Slovenia : [Faculty of Chemistry, Brno University of Technology, Brno, February 18, 2010]*. 2010; Brno. [COBISS.SI-ID 33741829]

KIŽ69. ŽGAJNAR GOTVAJN, Andreja, JUG, Aleš. *Faculty of Chemistry and Chemical Technology : study programmes and research work : [Norwegian University of Science and Technology (NTNU), 25th October 2010]*. Trondheim, 2010. [COBISS.SI-ID 34572549]

KIŽ70. PAVKO, Aleksander. *Fungal bioremediation : [École Polytechnique Féderale de Lausanne, EPFL, 18. October 2010]*. Lausanne, 2010. [COBISS.SI-ID 34556165]

UREDNIK / EDITORSHIP

KIŽ71. EFB Bioprocess Engineering Master Course, LIKOZAR, Blaž (ur.). *Abstracts*. [S. l.: s. n.], 2010. 1 optični disk (CD-ROM), barve. [COBISS.SI-ID 34492933]

KIŽ72. BEROVIČ, Marin (ur.), ENFORS, Sven-Olof (ur.). *Comprehensive bioprocess engineering : doctoral/post-doctoral*. Ljubljana: University, 2010. V, 444 str., graf. prikazi. ISBN 978-961-6410-28-1. [COBISS.SI-ID 252145664]

KIŽ73. International Thematic Conference Implementation of Microreactor Technology into Biotechnology, Ljubljana, September 29–30, 2010, ŽNIDARŠIČ PLAZL, Polona (ur.), CVJETKO, M. (ur.), POHAR, Andrej (ur.), STOJKOVIČ, Gorazd (ur.). *IMTB 2010 : [proceedings CD]*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2010. 1 optični disk (CD-ROM). ISBN 978-961-6756-20-4. [COBISS.SI-ID 252678656]

KIŽ74. *Acta chimica slovenica*. Levec, Janez (član uredniškega odbora 1998–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [COBISS.SI-ID 14086149]

KIŽ75. *Acta chimica slovenica*. Pavko, Aleksander (glavni urednik 2006–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [COBISS.SI-ID 14086149]

KIŽ76. *Biotechnology annual review*. Berovič, Marin (član uredniškega odbora 2002–). Amsterdam; Lausanne; New York; Oxford; Shannon; Tokyo: Elsevier. ISSN 1387-2656. [COBISS.SI-ID 23725061]

KIŽ77. *Chemical and biochemical engineering quarterly*. Plazl, Igor (urednik 2009–)Zagreb: Croatian Society of Chemical Engineers, 1987–. ISSN 0352-9568. [COBISS.SI-ID 49186]

KIŽ78. *Chemical and biochemical engineering quarterly*. Žnidaršič Plazl, Polona (članica uredniškega odbora 2009–). Zagreb: Croatian Society of Chemical Engineers, 1987–. ISSN 0352-9568. [COBISS.SI-ID 49186]

KIŽ79. Chinese journal of chemical engineering. Levec, Janez (član uredniškega sveta 2000–). Beijing: Chemical Industry Press; Heidelberg; New York; Tokyo: Springer-Verlag Berlin, 1982–. ISSN 1004-9541. [COBISS.SI-ID 2317850]

KIŽ80. European water management. Zagorc-Končan, Jana (član uredniškega odbora 1998–). Lavenham: Terence Dalton Publishers, 1998–. ISSN 1461-6971. [COBISS.SI-ID 1607450]

KIŽ81. International journal of chemical engineering. Levec, Janez (član uredniškega odbora 2008–). New York; Cairo: Hindawi Publishing Corporation. [COBISS.SI-ID 3883290]

KIŽ82. International review of chemical engineering. Levec, Janez (član uredniškega odbora 2009–). Napoli: Praise Worthy Prize. ISSN 2035-1755. [COBISS.SI-ID 4095514]

KIŽ83. Kemija u industriji. Plazl, Igor (član uredniškega odbora 2009–). [Print ed.]. Zagreb: Hrvatsko društvo kemijskih inženjera i tehnologa, 1952–. ISSN 0022-9830. [COBISS.SI-ID 747524]

KIŽ84. Phytomedicine. Berovič, Marin (član uredniškega odbora 2010–). Stuttgart; Jena; New York: Fischer, 1994–. ISSN 0944-7113. [COBISS.SI-ID 17566981]

KATEDRA ZA POLIMERNO INŽENIRSTVO, ORGANSKO KEMIJSKO TEHNOLOGIJO IN MATERIALE

CHAIR OF POLYMER ENGINEERING, ORGANIC CHEMICAL TECHNOLOGY AND MATERIALS

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Matjaž Krajnc

SODELAVCI KATEDRE / PERSONNEL

Učitelji /Faculty
prof. dr. Janvit Golob
prof. dr. Matjaž Krajnc

Asistenti / Assistants
doc. dr. Urška Šebenik

Raziskovalci / Researchers
dr. Jernej Kajtna
dr. Sergej Knez
dr. Igor Mihelič

Strokovni sodelavec / Research Assistant
Branko Alič, univ. dipl. kem.

Tehnik / Technician
Janez Malovrh

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Maja Šoštarič	J. Golob	2007–2012	doktorski študij / *PhD*
Ines Mohorič	U. Šebenik	2008–2013	doktorski študij / *PhD*
Ervin Šinkovec	M. Krajnc	2009–2013	doktorski študij / *PhD*
Miha Narobe	J. Golob	2010–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

Kemijsko inženirstvo / *Chemical Engineering* – UN:
Kemijsko inženirstvo I, II / *Chemical Engineering I, II*
Polimerni materiali (izbirni predmet) / *Polymer Materials (elective course)*

Kemijska tehnologija / *Chemical Technology* – VS:
Procesi v industrijski kemiji / *Processes in Industrial Chemistry*
Polimerni materiali (izbirni predmet) / *Polymer Materials (elective course)*
Osnove polimernega inženirstva (izbirni predmet) / *Principles of Polymer Engineering (elective course)*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Pregled tehnologij / *Principles of Technological Processes* – UN
Uvod v tehnologijo / *Introduction to Technology* – VS
Organski procesi in produkti / *Organic Processes and Products* – VS
Organska tehnologija I / *Organic Chemical Technology I* – UN
Polimeri / *Polymers* – UN
Separacijski procesi / *Separation Processes* – UN
Organski materiali in produkti / *Organic Materials and Products* – UN

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Izbrana poglavja iz separacijskih procesov / *Selected Topics in Separation Processes*
Izbrana poglavja iz polimernega inženirstva / *Selected Topics in Polymer Engineering*
Mehanika polimernih materialov / *Mechanics of Polymer Materials*

IZVEN FKKT / EXTRAMURAL COURSES

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Polimerna kemija I, II / *Polymer Chemistry I, II* NTF – UN

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

– Sinteza, karakterizacija in optimizacija procesa sinteze fenol-formeldehidnih smol, sečninsko-formaldehidnih smol, melaminsko-formaldehidnih smol, fenol-

sečninsko-formaldehidnih smol, melamin-sečninsko-formaldehidnih smol / *Synthesis, Characterization and Synthesis Process Optimization of Formaldehyde Resins*
- Tehnologija priprave melaminskih pen / *Technology for the Production of Melamine Foams*
- Inkapsulacija / *Encapsulation*
- Polisiloksanske emulzije na vodni osnovi / *Polysiloxane Water-Based Emulsions*
- Sinteza, karakterizacija in optimizacija procesa sinteze akrilatnih lepil / *Synthesis, Characterization and Synthesis Process Optimization of Acrylic Adhesives*
- Polimerizacijski procesi v mikroreaktorjih / *Polymerization Processes in Microreactors*
- Sinteza, priprava in karakterizacija nanokompozitnih materialov / *Synthesis, Preparation and Characterization of Nanocomposite Materials*
- Funkcionalizacija in vulkanizacija gumenih zmesi / *Functionalization and Vulcanization of Rubber Blends*
- Mehanske lastnosti polimernih materialov in kompozitov / *Mechanical Properties of Polymer Materials and Composites*
- Membransko oplaščanje umetnih gnojil s podaljšanim delovanjem / *Preparation of Polymer-Coated Fertilizers with Controlled Release*
- Sinteza kelatov za agrokemijske namene / *Chelate Synthesis for Agrochemical Purposes*
- Študij adsorpcije biocidov v praškastih formulacijah / *Biocide Adsorption in Powder Formulations for Agrochemical Purposes*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Mettler Toledo DMA 861e
- Mettler Toledo DSC 1
- Mettler Toledo ReactIR iC10
- Perkin Elmer FTIR Spectrum 1000
- HP 5980II Gas Chromatograph
- LC Shimadzu LC-4A
- Microtrac S 3500 Laser Particle Size Analyzer
- Brabender Plastograph EC »PLUS«
- 3D-DLS Research Lab
- Mettler Toledo LabMax Automatic Lab Reactor

SODELOVANJE V TEHNOLOŠKIH MREŽAH IN PLATFORMAH / TECHNOLOGY NETWORKS & PLATFORMS

- Tehnološka mreža: Inteligentni polimerni materiali in pripadajoče tehnologije / *Technology Network: Intelligent Polymer Materials and Technologies*
- Tehnološka platforma NaMaT: Napredni materiali in tehnologije / *Technology Platform NaMaT: Advanced Materials and Technologies*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P2–0191	Kemijsko inženirstvo / *Chemical Engineering* Vodja programa / *Principal Researcher:* M. Krajnc
P2–0346	Separacijski procesi toplogrednih plinov za trajnostni razvoj / *Separation Processes of Greenhouse Gases for Sustainable Development* Vodja programa / *Principal Researcher:* J. Golob

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

Inkapsulacija / *Encapsulation*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Melamin d.d.

Raziskave in razvoj na področju melaminskih pen / *Research and Development of Melamine Foams*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Melamin d.d.

Oplaščanje umetnih gnojil s podaljšanim delovanjem, sinteza kelatov in adsorpcija biocidov v praškastih formulacijah za agrokemijske namene / *Preparation of Polymer-Coated Controlled-Release Fertilizers, Chelate Synthesis, and Study of Biocide Adsorption in Powder Formulations for Agrochemical Purposes*
Nosilec / *Principal Researcher*: J. Golob
Financer / *Sponsored by*: Unichem d.o.o.

Raziskave na področju naftnih derivatov / *Oil Derivatives Research*
Nosilec / *Principal Researcher*: J. Golob
Financer / *Sponsored by*: Nafta Lendava d.o.o.

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Madžarska *Slovenia – Hungary*	Kompoziti guma / poliuretan /nanopolnilo: Struktura in lastnosti / *Rubber / Polyurethane / Nanofiller Systems: Structure and Properties* Nosilka / *Principal Researcher*: U. Šebenik

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

POT1. ŠREKL, Jože, GOLOB, Janvit. Impact of the buildings areas on the fire incidence. *Acta chim. slov.*, 2010, vol. 57, no. 1, str. 118–122. [COBISS.SI-ID 33808645]

POT2. KLOFUTAR, Boštjan, GOLOB, Janvit, LIKOZAR, Blaž, KLOFUTAR, Cveto, ŽAGAR, Ema, POLJANŠEK, Ida. The transesterification of rapeseed and waste sunflower oils : mass-transfer and kinetics in a laboratory batch reactor and in an industrial-scale reactor/separator setup. *Bioresour. technol.*, 2010, vol. 101, no. 10, str. 3333–3344. [COBISS.SI-ID 33677317]

POT3. KAJTNA, Jernej, KRAJNC, Matjaž. UV crosslinkable microsphere pressure sensitive adhesives : influence on adhesive properties. *Int. j. adhes. adhes.*, doi: 10.1016/j.ijadhadh.2010.09.004. [COBISS.SI-ID 34530309]

POT4. ALIČ, Branko, ŠEBENIK, Urška, KRAJNC, Matjaž. Differential scanning calorimetric examination of melamine-formaldehyde microcapsules containing decane. *J. appl. polym. sci.*, doi: 10.1002/app.33077. [COBISS.SI-ID 34469637]

POT5. MOHORIČ, Ines, ŠEBENIK, Urška. Anionic ring-opening polymerization of octamethylcyclotetrasiloxane in emulsion above critical micelle concentration. *Polymer*, doi: 10.1016/j.polymer.2011.01.025. [COBISS.SI-ID 34739717].

PREGLEDNI ZNANSTVENI ČLANEK / REVIEW ARTICLE

POT6. PODGORNIK, Aleš, JANČAR, Janez, MIHELIČ, Igor, BARUT, Miloš, ŠTRANCAR, Aleš. Large volume monolithic stationary phases : preparation, properties, and applications. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 1–8. [COBISS.SI-ID 3772536]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

POT7. ALIČ, Branko, ŠEBENIK, Urška, KRAJNC, Matjaž. Microencapsulation with melamine-formaldehyde resin. V: 14th European Conference on Composite Materials, 7–10 June, Budapest, Hungary. *Proceedings : ECCM14*. [S. l.: s. n.], 2010, str. 1–9. [COBISS.SI-ID 34553861]

POT8. BERCE, Peter, GOLOB, Janvit, LIKOZAR, Blaž. Rast mikroalge Chlorella vulgaris pod različnimi svetlobnimi režimi = Growth of microalgae Chlorella vulgaris under different exposures to light. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–6. [COBISS.SI-ID 34476805]

POT9. PIVAR, Robert, GOLOB, Janvit, LIKOZAR, Blaž. Analiza tehnoloških procesov od parnega reforminga do proizvodnje formaldehida = Analysis of technological processes from steam reforming to formaldehyde production. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–8. [COBISS.SI-ID 34476293]

POT10. LAPORNIK, Domen, GOLOB, Janvit, LIKOZAR, Blaž. Ravnotežje in prenos snovi pri sušenju agarnih gelov za pripravo rodenticida = Equilibrium and mass transfer during drying of agar gels for rodenticide preparation. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–10. [COBISS.SI-ID 34471173]

POT11. KAVŠEK, Miha, GOLOB, Janvit, LIKOZAR, Blaž. Mikroenkapsulacija insekticida s polisečnino = Microencapsulation of insecticide with polyurea. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–11. [COBISS.SI-ID 34476549]

POT12. NOGRAŠEK, Boštjan, KOZLEVČAR, Bojan, GOLOB, Janvit, LIKOZAR, Blaž. Načrtovanje integriranega procesa oplaščanja zrn umetnih gnojil in sušenja v fluidiziranem sloju = Design of integrated process of synthetic fertilizer coating process and drying in fluidized bed. V: *Slovenski kemijski dnevi 2010, Maribor, 23. in 24. september 2010*. [Maribor]: FKKT, [2010], str. 1–11. [COBISS.SI-ID 34477061]

POT13. PRINČIČ, Tina, GOLOB, Janvit, STRUPI-ŠUPUT, Jerneja, KOGLOT, Karmen, COTIČ, Zvonko. Vpliv dodatka superplastifikatorja in elektrofiltrskega pepela na lastnosti cementnih malt. V: Konferenca Beton 21. stoletja, Lipica, marec 2010. *Zbornik referatov*. Ljubljana: ZBS, Združenje za beton Slovenije, 2010, str. 48–57, ilustr. [COBISS.SI-ID 33876229]

SAMOSTOJNI ZNANSTVENI SESTAVEK ALI POGLAVJE V MONOGRAFSKI PUBLIKACIJI / INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

POT14. ŠEBENIK, Urška, KRAJNC, Matjaž. Acrylic-clay nanocomposites by suspension and emulsion polymerization. V: MITTAL, Vikas (ur.). *Polymer nanocomposites by emulsion and suspension polymerization*, (RSC nanoscience & nanotechnology, no. 16). Cambridge: RSC Pub., cop. 2011, str. 111–123. [COBISS.SI-ID 34554629]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

POT15. ŠEBENIK, Urška. *Polimerna kemija : Elektronski vir : interno študijsko gradivo za študente 3. letnika univerzitetnega študijskega programa Materiali*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo in organsko kemijsko tehnologijo, 2010. 1 el. optični disk (256 str.), ilustr. [COBISS.SI-ID 33856773]

POT16. ŠEBENIK, Urška. *Polimerni materiali : Elektronski vir : interno študijsko gradivo za študente 2. letnika visokošolskega študijskega programa Kemijska tehnologija*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 1 el. optični disk (160 str.), ilustr. [COBISS.SI-ID 34678021]

POT17. ŠEBENIK, Urška. *Procesi v industrijski kemiji: organski del : Elektronski vir : interno študijsko gradivo za študente 2. letnika visokošolskega študijskega programa Kemijska tehnologija*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 1 el. optični disk (97 str.), ilustr. [COBISS.SI-ID 34677765]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

POT18. GOLOB, Janvit, LIKOZAR, Blaž, PIVAR, Robert, BENCIK, Dejan, PEČELIN, Peter. *Analiza tehnološkega procesa proizvodnje formaldehida po metaloksidnem postopku : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 24 f., ilustr. [COBISS.SI-ID 34520837]

POT19. KRAJNC, Matjaž, ŠEBENIK, Urška, ALIČ, Branko. *Inkapsulacija butil stearata z melaminsko-formaldehidno smolo : poročilo o delu po pogodbi R001/2010 za MELAMIN d.d. Kočevje*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 68 f., ilustr. [COBISS.SI-ID 34386437]

POT20. GOLOB, Janvit, LIKOZAR, Blaž, KOZLEVČAR, Bojan, FRANCETIČ, Vojmir, NOGRAŠEK, Boštjan, DEVETAK, Marko. *Razvoj tehnologij enkapsulacije gnojil : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 22 f., ilustr. [COBISS.SI-ID 34475269]

POT21. GOLOB, Janvit, LIKOZAR, Blaž, KAVŠEK, Miha, MATJAŠIČ, Aleš, DEVETAK, Marko. *Razvoj tehnologij mikroenkapsulacije pesticidov : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 29 f., ilustr. [COBISS.SI-ID 34448645]

POT22. GOLOB, Janvit, LIKOZAR, Blaž, LAPORNIK, Domen, DEVETAK, Marko. *Razvoj tehnologij rodenticidov : vmesno poročilo*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 28 f., ilustr. [COBISS.SI-ID 34467077]

POT23. KRAJNC, Matjaž, ŠEBENIK, Urška, ALIČ, Branko. *Vmesno poročilo o laboratorijskih raziskavah : ZI 1.1.1.3 poročilo o raziskavah kemizma reakcije in reologije : poročilo o delu po pogodbi z dne 30.9.2009 za MELAMIN kemična tovarna d.d. Kočevje : predmet pogodbe: RR sodelovanje v okviru projekta RIP 09-11 : ob mejniku M2, 15.01.2010*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, 2010. 14 f., ilustr. [COBISS.SI-ID 33635845]

POT24. KRAJNC, Matjaž, ŠEBENIK, Urška, ALIČ, Branko. *Vmesno poročilo o laboratorijskih raziskavah : ZI 1.1.1.3 poročilo o raziskavah sestavin reakcijske mešanice : poročilo o delu po pogodbi z dne 30.9.2009 za MELAMIN kemična tovarna d.d. Kočevje : predmet pogodbe: RR sodelovanje v okviru projekta RIP 09-11 : ob mejniku M2, 15.01.2010*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, 2010. 28 f., ilustr. [COBISS.SI-ID 33636613]

POT25. KRAJNC, Matjaž, ŠEBENIK, Urška, ALIČ, Branko. *Vmesno poročilo o raziskavah aplikativne uporabe melaminskih pen : poročilo o delu po pogodbi z dne 30.9.2009 za MELAMIN kemična tovarna d.d. Kočevje : predmet pogodbe: RR sodelovanje v okviru projekta RIP 09-11 : ob mejniku M2, 15.01.2010*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, 2010. 10 f., ilustr. [COBISS.SI-ID 33636101]

POT26. KRAJNC, Matjaž, ŠEBENIK, Urška, ALIČ, Branko. *Vpliv procesnih pogojev na strukturo in zamreževanje sečninsko-formaldehidnih smol : zaključno poročilo o delu po pogodbi KPIOT-2/2008 za NAFTO – Petrochem d.o.o.*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za polimerno inženirstvo, organsko kemijsko tehnologijo in materiale, 2010. 116 f., graf. prikazi. [COBISS.SI-ID 34479621]

PATENTNA PRIJAVA / PATENT APPLICATION

POT27. OSMAK, Maja, POLANC, Slovenko, ČIMBORA, Tamara, BROZOVIĆ, A., KOČEVAR, Marijan, MAJCE, Vita, ALIČ, Branko. *Analogues of 1, 3-bis(4-nitrophenyl)triazenes, their pharmaceutically acceptable salts and N-acyl derivatives for tumor treatment : patentna prijava : WO 2010103338 (A1), 2010-09-16*. [S. l.]: World Intellectual Property Organization, 2010. 21 str., ilustr. [COBISS.SI-ID 30639621]

UREDNIK / EDITORSHIP

POT28. GOLOB, Janvit (ur.), TRATNIK-VOLASKO, Marjeta (ur.). *Kaj lahko pričakujemo od centrov odličnosti?*, (Zbornik referatov in razprav, 2010, št. 1). Ljubljana: Državni svet Republike Slovenije, 2010. 75 str., graf. prikazi, tabele. ISBN 978-961-6453-34-9. [COBISS.SI-ID 250476032]

POT29. GOLOB, Janvit (ur.), TRATNIK-VOLASKO, Marjeta (ur.). *Nacionalna strategija razvoja energetike na področju tekočih goriv v okviru zelene knjige*, (Zbornik referatov in razprav, 2010, št. 2). Ljubljana: Državni svet Republike Slovenije, 2010. 42 str. ISBN 978-961-6453-35-6. [COBISS.SI-ID 250895872]

KATEDRA ZA VARSTVO PRI DELU
CHAIR OF SAFETY AT WORK

PREDSTOJNIK KATEDRE / HEAD

dr. Jože Šrekl

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
doc. dr. Mitja Robert Kožuh
dr. Jože Šrekl, viš. pred.
mag. Aleš Jug, pred.

v dopolnilnem razmerju / *part time*
prof. dr. Stojan Petelin
doc. dr. Marija Molan

Asistent / Assistant
Marjan Lukežič, univ. dipl. inž.

Tehnika / Technicians
Iztok Košir
Miran Banfi

Administrativno osebje / Administration
Slavka Lobnik

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Bolonjski program 1. stopnje / *Bologna 1st Cycle Study Programme*

Tehniška varnost / *Technical Safety* – UN:
Osnove zdravstvenega varstva / *Fundamentals of Health Care*
Osnove tehniške in požarne varnosti / *Fundamentals of Technical and Fire Safety*
Varnost v strojništvu / *Safety in Mechanical Engineering*
Strojni in gradbeni elementi / *Machine and Construction Elements*
Numerične metode v varnosti I / *Numerical Methods in Safety I*

Bolonjski program 2. stopnje / *Bologna 2nd Cycle Master Study Programme*

Tehniška varnost / *Technical Safety*:
Numerične metode v varnosti II / *Numerical Methods in Safety II*
Vodenje tveganja in procesna varnost / *Risk Management and Process Safety*
Varno projektiranje in ranljivost sistemov / *Safe Design and Vulnerability of Systems*
Intervencije in reševanje / *Interventions and Rescue*
Človeški in organizacijski dejavniki / *Human and Organizational Factors*

Predbolonjski dodiplomski program / *Pre- Bologna Professional Study Programme*

Psihologija dela / *Occupational Psychology* – VS
Varstvo okolja II / *Environmental Protection II* – VS
Medicina in higiena dela / *Medicine and Occupational Hygiene* – VS
Ergonomija in ergonomske meritve / *Ergonomics and Ergonomic Measurements* – VS
Varnost delovnih priprav in naprav / *Safety of Machinery and Equipment* – VS
Gašenje požarov in reševanje / *Fire Fighting and Rescue* – VS

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

- Nove metodologije ocenjevanja tveganja / *New Methods in Risk Assessment*
- Ocenjevanje kompleksnih tehnoloških sistemov / *Assessment of Complex Techological Systems*
- Človek – element tveganja / *Human as a Risk Factor*
- Metodologija statistike požarov /*Methodology of Fire Statistics*
- Inženirske metode pri vrednotenju požarne varnosti / *Engineering Methods in Fire Safety Assessment*
- Modeliranje s strukturnimi enačbami v oceni požarne ogroženosti / *Structural Equation Modelling in Fire Risk Assessment*

– Problemsko zasnovan študij na področju statistike / *Problem-Based Learning in Statistics*
– Razvoj simulatorja cestnega predora za usposabljanje operabilnega osebja v nadzornem centru / *Development of Road Tunnel Simulator for Training of Staff in Operation Control Center*
– Analiza dejanskega požara v predoru Trojane / *Analysis of Actual Fire in the Trojane Tunnel*
– Varnostna analiza predora Karavanke / *Safety Analysis of Karavanke Tunnel*
– Analize tveganj nekaterih slovenskih cestnih predorov / *Risk Analysis of Some Road Tunnels in Slovenia*
– Analize varnosti načrtovanih plinskih terminalov v Tržaškem zalivu / *Safety Analysis of LNG Terminals Planned in the Gulf of Trieste*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

– David Levovnik, Nagrada Avgusta Kuharja za najboljše diplomsko delo za leto 2010 / *The Avgust Kuhar Award for the Best Diploma Thesis in 2010*
– M. Kožuh, pohvala Študentskega sveta za pedagoško delo na smeri Tehniška varnost / *Students Award for the Quality of Teaching in Technical Safety Study Programme*

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL MEETINGS

– Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož, maj 2010 / *Safety at Work, Fire Safety and Occupational Medicine, Two-day Symposium with International Participation, Portorož, May 2010*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L2–2324 Optimizacija upravljanja cestnih predorov med normalnimi in izrednimi razmerami / *Optimizing the Management of Road Tunnels during Normal and Emergency Situations*
Nosilec / *Principal Researcher:* S. Petelin (UL FPP)
Sofinancer / *Co-sponsored by*: DARS d.d. – Družba za avtoceste RS

BIBLIOGRAFIJA 2010 / REFERENCES 2010

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

VP1. ŠREKL, Jože, GOLOB, Janvit. Impact of the buildings areas on the fire incidence. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 118–122. [COBISS.SI-ID 33808645]

VP2. LUKEŽIČ, Marjan, MARINŠEK, Marjan, FAGANELI, Jadran. Evaluation of burning test rate method for flammable solids to increase air-cargo safety. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 129–135. [COBISS.SI-ID 33808901]

VP3. JUG, Aleš, PETELIN, Stojan, BUKOVEC, Peter. Designing an underground car park fire scenarios on a probabilistic basis. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 136–143. [COBISS.SI-ID 33809157]

VP4. MOLAN, Marija, MOLAN, Gregor. Model izboljšanja psihičnega funkcioniranja v delovnem okolju = Model of the improvement of mental functioning in the working environment. *Sanitas et labor*, apr. 2010, letn. 8, št. 1, str. 23–38. [COBISS.SI-ID 26811609]

VP5. PETELIN, Stojan, LUIN, Blaž, VIDMAR, Peter. Risk analysis methodology for road tunnels and alternative routes. *Stroj. vestn.*, 2010, vol. 56, no. 1, str. 41–51. [COBISS.SI-ID 2059363]

VP6. PERKOVIČ, Marko, PETELIN, Stojan, HARSCH, Rick. Hindcast simulation and data fusion: satellite technology applied to illict pollution at sea = Szmulacja oparta na danych historycznych i dane »fusion«: satelitarna technologia stosowana do wykrycia nielegalnych zanieczyczczeń na morzu. *Zesz. Nauk. (Akad. Mor. Szczec.)*, 2010, vol. 20, no. 92, str. 107–113. [COBISS.SI-ID 2090595]

PREGLEDNI ZNANSTVENI ČLANEK / REVIEW ARTICLE

VP7. KOŽUH, Mitja. The Seveso II Directive in new european member states : the case of Slovenia. *Acta chim. slov.*. [Tiskana izd.], 2010, vol. 57, no. 1, str. 17–28. [COBISS.SI-ID 33794565]

VP8. MOLAN, Marija. Strateški cilj humanega delovnega okolja : psihično zdravje na delovnem mestu. *Delo + varnost*, 2010, letn. 55, št. 2, str. 22–27, ilustr. [COBISS.SI-ID 11357979]

VP9. MOLAN, Marija, MOLAN, Gregor. Vpliv delovnega časa na počutje in razpoložljivost. *Delo + varnost*, 2010, letn. 55, št. 4, str. 10–19, ilustr. [COBISS.SI-ID 11493915]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

VP10. VIDMAR, Peter, PETELIN, Stojan, PERKOVIČ, Marko. Approach in risk assessment for LNG terminals. V: GELDER, Pieter van (ur.), GUCMA, Lucjan (ur.), PROSKE, Dirk (ur.). *Proceedings of the 8th International probabilistic workshop, Szczecin, 18–19 november 2010*. Szczecin: Akademia Morska, 2010, 2010, str. 355–376. [COBISS.SI-ID 2130275]

VP11. PERKOVIČ, Marko, GUCMA, Lucian, PRZYWARTY, Marcin, GUCMA, Lucjan, PETELIN, Stojan. Nautical risk assessment for LNG operations at the Port of Koper. V: ZANNE, Marina (ur.), BAJEC, Patricija (ur.). *Promet, pomorstvo in logistika : zbornik referatov : conference proceedings*. Portorož: Fakulteta za pomorstvo in promet, 2010, 2010, 11 str. [COBISS.SI-ID 2092643]

VP12. VIDMAR, Peter, PETELIN, Stojan, PERKOVIČ, Marko. Approach in risk assessment for LNG terminals. V: ANŽEK, Mario (ur.), HERNAVS, Boštjan (ur.), KAVRAN, Zoran (ur.), MEŠE, Pavel (ur.), ŠTERN, Andrej (ur.). 18th International Symposium on Electronics in Traffic, ISEP 2010, March 29, 2010, Ljubljana. *The role of ITS in the near future : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2010, 2010, p13 [10 f.]. [COBISS.SI-ID 2062947]

VP13. CVETKOVIĆ, Martina, PETELIN, Stojan, KOŽUH, Mitja. Surveillance and control of LNG terminal. V: ANŽEK, Mario (ur.), HERNAVS, Boštjan (ur.), KAVRAN, Zoran (ur.), MEŠE, Pavel (ur.), ŠTERN, Andrej (ur.). 18th International Symposium on Electronics in Traffic, ISEP 2010, March 29, 2010, Ljubljana. *The role of ITS in the near future : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2010, f. [1–4]. [COBISS.SI-ID 33865477]

VP14. JUG, Aleš, PETELIN, Stojan, BUKOVEC, Peter. Correlation of underground car park impulse ventilation control and realistic fire scenarios. V: ANŽEK, Mario (ur.), HERNAVS, Boštjan (ur.), KAVRAN, Zoran (ur.), MEŠE, Pavel (ur.), ŠTERN, Andrej (ur.). 18th International Symposium on Electronics in Traffic, ISEP 2010, March 29, 2010, Ljubljana. *The role of ITS in the near future : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2010, f. [1–7]. [COBISS.SI-ID 33865221]

VP15. LUIN, Blaž, PETELIN, Stojan. Road tunnel emergency response simulator. V: ANŽEK, Mario (ur.), HERNAVS, Boštjan (ur.), KAVRAN, Zoran (ur.), MEŠE, Pavel (ur.), ŠTERN, Andrej (ur.). 18th International Symposium on Electronics in Traffic, ISEP 2010, March 29, 2010, Ljubljana. *The role of ITS in the near future : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2010, 2010, str. R2. [COBISS.SI-ID 2063203]

VP16. ŠREKL, Jože. Uporaba normalne in log-normalne porazdelitve pri oceni rezultatov meritev delovnega okolja. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2010, 11.–12. 5. 2010*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2010, str. [1–6]. [COBISS.SI-ID 34041093]

VP17. LUKEŽIČ, Marjan. Čas vžiga – pomemben parameter pri razvrščanju trdnih vnetljivih snovi. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2010, 11.–12. 5. 2010*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2010, str. 1–9. [COBISS.SI-ID 34041605]

VP18. KOŽUH, Mitja. Vpliv vzdrževanja na varnost. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2010, 11.–12. 5. 2010*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2010, str. [1–9]. [COBISS.SI-ID 34040581]

VP19. JUG, Aleš. Požari v podzemnih garažnih hišah. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2010, 11.–12. 5. 2010*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2010, str. [1–12]. [COBISS.SI-ID 34043653]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

VP20. ŽGAJNAR GOTVAJN, Andreja, JUG, Aleš. Faculty of Chemistry and Chemical Technology : study programmes and research work : [Norwegian University of Science and Technology (NTNU), 25th October 2010]. Trondheim, 2010. [COBISS.SI-ID 34572549]

UREDNIK / EDITORSHIP

VP21. MOLAN, Marija (ur.), DODIČ-FIKFAK, Metoda (ur.). *Izbrane teme o duševnem zdravju*, (Sanitas et labor, letn. 8, št. 1). Ljubljana: Univerzitetni klinični center, Klinični inštitut za medicino dela, prometa in športa: = University Medical Centre, Institute of Occupational, Traffic and Sports Medicine, 2010. 156 str., [ilustr.]. ISBN 978-961-91429-9-8. [COBISS.SI-ID 250430208]

VP22. *Sanitas et labor*. Molan, Marija (odgovorni urednik 2001–). Ljubljana: Klinični inštitut za medicino dela prometa in športa, Združenje za medicino dela, prometa in športa, 2001–. ISSN 1580-5972. [COBISS.SI-ID 111898368]

POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2010

Izdala: Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani

Avtorji prispevkov: Anton Meden, Marija Bešter Rogač, Peter Bukovec, Marko Dolinar, Andrej Godec, Janvit Golob, Marijan Kočevar, Ksenija Kogej, Matjaž Krajnc, Maja Lamovšek, Ivan Leban, Brigita Lenarčič, Slavka Lobnik, Jadran Maček, Zdenka Modic, Stojka Oman Vučkovska, Aleksander Pavko, Andrej Petrič, Boris Pihlar, Dominika Slabajna, Branko Stanovnik, Jurij Svete, Boris Šket, Jože Šrekl, Janez Topovšek, Iztok Turel, Marjan Veber, Vojeslav Vlachy, Klementina Zupan, Polona Žnidaršič Plazl

Uredila: Miloš Komac, Stojka Oman Vučkovska
Lektorica (angl): Nada Vukadinovič
Fotografije: Aleš Gregorič, Uroš Novak, Iztok Turel, Andrej Godec, Goran Miličić
Oblikovanje: Studio Signum
Tisk: Birografika Bori
Naklada: 250 izvodov

ISSN 1855-0193