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

# POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2009

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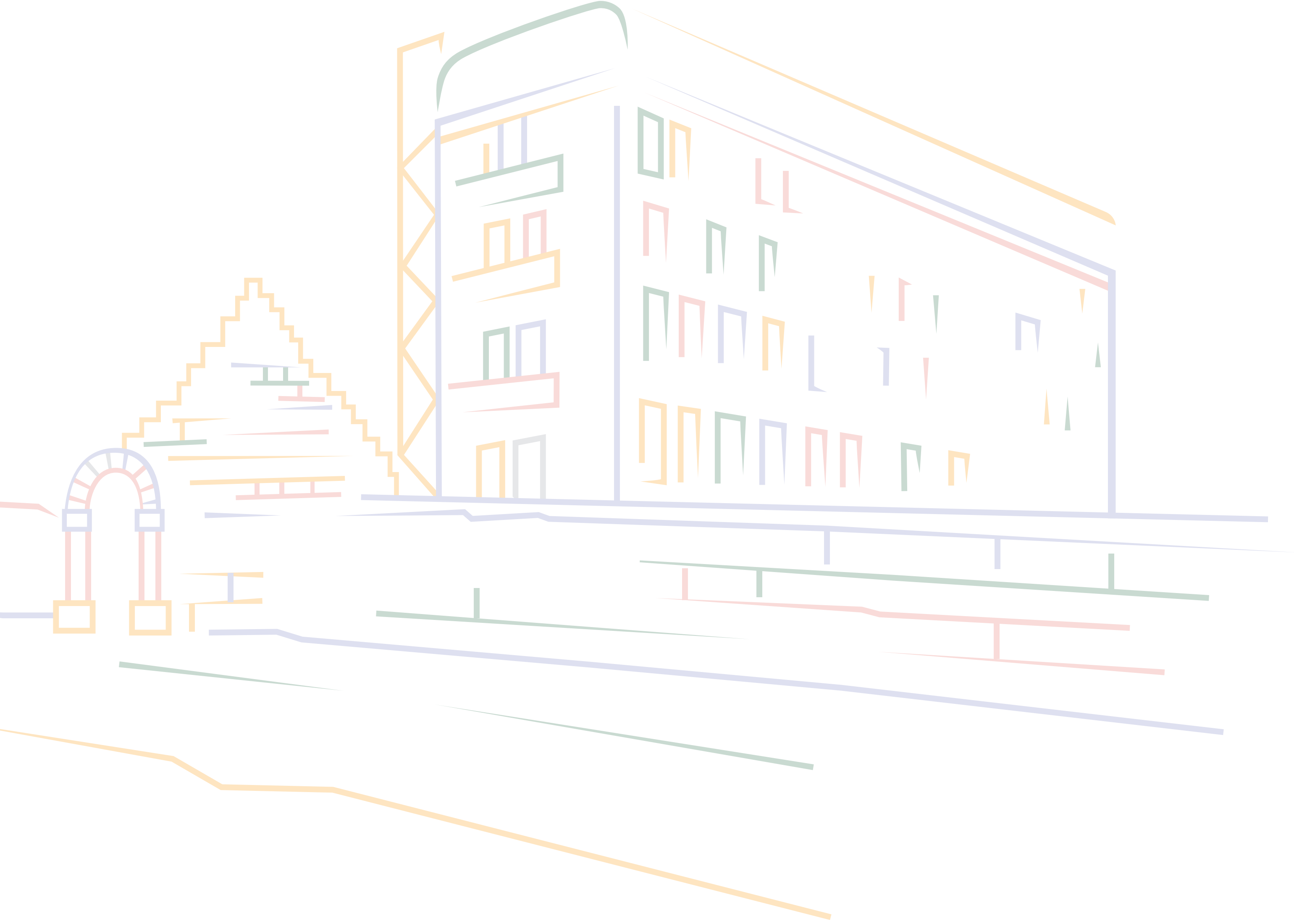
# *ANNUAL REPORT 2009*



Ljubljana, 2010

# KAZALO

# UVODNA BESEDA

Poročilo o izobraževalni in raziskovalni dejavnosti v letu 2009, ki ga prebirate, opisuje delo in dosežke sodelavcev Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani (FKKT UL) v jubilejnem letu praznovanja 90-letnice kemijskih študijev na UL. V marsičem se to leto ne razlikuje veliko od preteklih let, saj se trudimo vzdrževati in po možnosti izboljševati kakovost našega pedagoškega in raziskovalnega dela. Rad pa bi omenil nekaj dosežkov, ki so za leto 2009 posebni.

Pedagoško delo je v letu 2009 dobilo novo obliko. Po uspešni akreditaciji enajstih bolonjskih študijskih programov, od tega petih prvostopenjskih, petih drugostopenjskih in enega tretjestopenjskega, smo tudi prvič vpisali študente v vse prenovljene prvostopenjske programe in doktorski program. Študij prve generacije študentov skrbno spremljamo in poskušamo sproti reševati težave, ki se pojavljajo, zato verjamem, da bomo skupaj s študenti uspešno preorali ledino. Vabljena predavanja vrhunskih znanstvenikov, ki smo jih organizirali v okviru doktorskega študija, so upravičila naša visoka pričakovanja, saj se študenti tretje stopnje na ta način iz prve roke seznanijo z najnovejšimi dosežki na področju kemijskih znanosti.

Na področju raziskovalnega dela smo veseli pridobitve dveh novih instrumentov, NMR spektrometra in elektronskega mikroskopa, v skupni vrednosti približno 1,2 milijona evrov. S tem so ob vključitvi nekaj že obstoječih večjih kosov raziskovalne opreme postavljeni temelji infrastrukturnega centra fakultete, ki bo združeval in zagotavljal delovanje in dostopnost večje raziskovalne opreme za sodelavce FKKT, pa tudi širše. Dostop do kvalitetne raziskovalne opreme, ki je pogoj za uspešno znanstveno delo, smo si v precejšnji meri zagotovili tudi z vključenostjo naših raziskovalcev v štiri centre odličnosti.

V letu 2009 so se intenzivno nadaljevali postopki, povezani z gradnjo nove stavbe. Projekt je pridobil končno soglasje Vlade RS, prva faza, izgradnja mostu čez Glinščico, pa je v tem letu prišla do izbire izvajalca, ki je most začel graditi v letu 2010.

Vsem sodelavcem Fakultete za kemijo in kemijsko tehnologijo se iskreno zahvaljujem za uspešno delo, ki je pripeljalo do lepih rezultatov in potrdilo visoko kakovost delovanja fakultete. Prepričan sem, da bomo s skupnim zavzetim delom tudi v prihodnje skrbeli za uspešnost in ugled FKKT UL.

Meden

Dekan:
prof. dr. Anton Meden

# FOREWORD

*This annual report presents the achievements of the Faculty of Chemistry and Chemical Technology, University of Ljubljana (FKKT UL) gained through educational and research activities in 2009. This year was also marked by the celebration of the 90th anniversary of chemistry studies at the University of Ljubljana.*

*It may seem that last year was not much different from previous years. This is because we have always strived to maintain high quality level of our pedagogical and research work, and even improved it. However, I would like to highlight some events which have brought significant changes to our work.*

*The main change refers to our pedagogical work which assumed a new form: After obtaining accreditation for eleven study programmes according to the Bologna reform, the first generation of students was enrolled in the first year of studies. This includes five first-cycle programmes and one third-cycle programme. Since this was a completely new experience for us it will require careful monitoring throughout the year, and I believe that together with students we will manage to eliminate any problems arising. For the third-cycle programme we managed to organise invited lectures for doctoral students, delivered by eminent professionals. This form proved to meet our expectations since in this way students could receive first-hand information on scientific developments in the area of chemical sciences.*

*Our researchers have been particularly glad to obtain two pieces of new equipment: a NMR spectrometer and electron microscope, at the total value of 1.2 million Euros. Together with the existing research equipment we have laid foundations for the infrastructural centre of the Faculty which will offer access to research equipment to the faculty staff, as well as other users. We are aware that access to high quality research equipment is a prerequisite for serious scientific work. Our own equipment is complemented with the equipment from four centres of excellence in which our researchers are engaged.*

*In 2009 the Faculty was intensely working on the project of building our new premises. We managed to obtain an agreement from our government for construction developments. The first phase involved selecting a contractor for building a bridge across the Glinščica river and the works have already started.*

*Merits for our success and achievements go to all Faculty staff and therefore the contributions of each of them are greatly acknowledged. With their dedicated work each has contributed to the overall success of our institution which brought fine results and proved again that we can keep up with high quality standards. I firmly believe that with dedication and joint efforts of the team, we will be able to continue to maintain high standards of work and care for the reputation of FKKT UL in the future as well.*

Meden

*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 (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, usnjarsko-predelovalne 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

V letu 2009 se je na FKKT izvajalo pet 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 FKKT sodelovala z drugimi fakultetami pri izvajanju naslednjih podiplomskih študijskih programov:

- Biomedicina za področje Biokemije in molekularne biologije
- Biotehnologija
- Materiali
- Varstvo okolja

V študijskem letu 2009/10 smo prvič vpisali študente na prenovljene univerzitetne prvostopenjske programe Kemija, Biokemija, Kemijsko inženirstvo in Tehniška varnost, na prvostopenjski visokošolski strokovni program Kemijska tehnologija ter na prenovljeni doktorski program Kemijske znanosti.

Pri Svetu Republike Slovenije za visoko šolstvo so akreditirani tudi drugostopenjski programi Kemija, Biokemija, Kemijsko inženirstvo, Tehniška varnost in Kemijsko izobraževanje. V šolskem letu 2009/10 bomo tako prvič izvajali drugostopenjski program Tehniške varnosti.

Za izvedbo študijskih programov skrbi 32 rednih profesorjev, 17 izrednih profesorjev, 5 docentov, 2 višja predavatelja, 1 predavatelj, 51 asistentov, 3 strokovni sodelavci 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 inštitucijami, ter mednarodne povezave v sklopu mednarodnih projektov in sodelovanja s tujimi univerzami ali raziskovalnimi laboratoriji.

## 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 2009 je bilo na izmenjavi v tujini, za študij in prakso, 20 naših študentov, iz tujine pa smo imeli na izmenjavi eno študentko. 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 izmenjave študentov Erasmus Mundus Basileus, ki omogoča izmenjave študentov v in iz JV Evrope. V okviru tega programa sta bila v letu 2009 pri nas na izmenjavi dva doktorska študenta iz Srbije.

Na raziskovalnem področju poteka sodelovanje pri številnih dvostranskih projektih. V letu 2009 je Fakulteta za kemijo in kemijsko tehnologijo sodelovala pri 19 bilateralnih projektih z 12 državami. Na področju raziskovalnega dela na projektih COST sodeluje fakulteta pri šestih projektih.

V okviru projektov Evropske Unije, 6. in 7. Okvirnega programa, se je en projekt v letu 2009 končal, en projekt pa je še v teku. V okviru projektov VŽU poteka raziskovalni projekt Leonardo da Vinci – prenos inovacij.

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

# VKLJUČENOST V OKOLJE

## KEMIJSKA OLIMPIJADA 2009 V CAMBRIDGEU

Slovenska ekipa dijakov se je udeležila 41. Mednarodne kemijske olimpijade, ki je potekala od 18. 7. do 27. 7. 2009 v Veliki Britaniji.

Našo državo so zastopali Nika Anžiček (gimnazija Brežice), Marija Malgaj (gimnazija Celje), Luka Andrejčič (gimnazija Novo mesto) in Jernej Repas (gimnazija Slovenj Gradec). Mentorja ekipe pa sva bila mag. Breda Novak in dr. Andrej Godec.

Organizacijo letošnje olimpijade sta si delili dve sloviti univerzi: Cambridge in Oxford. Dijaki so ves čas olimpijade preživeli v Cambridgeu; nastanili so jih v Trinity College. Mentorji smo prve štiri dni preživeli v Oxfordu, potem pa smo se preselili v Cambridge. Univerza Cambridge letos praznuje 800 let obstoja, tako da je bila tudi olimpijada v znamenju te obletnice.

Obe mesti nosita močan pečat univerz. Oxford ima sicer 300 000 prebivalcev, Cambridge pa je s svojimi 130 000 prebivalci veliko manjši.

Dijaki imajo dva tekmovalna dneva. Najprej je na vrsti praktični del, ki ga izvajajo v laboratoriju. V petih urah so morali letos izvesti tri eksperimente: aldolno kondenzacijo brez prisotnosti topil, titrimetrično analizo bakrovega kompleksa, in konduktometrično določitev kritične micelne koncentracije surfaktanta natrijevega dodecil sulfata.

Čez dva dni je na vrsti teoretični test. Letos je bil sestavljen iz šestih nalog: tri so bile iz področja fizikalne kemije, ostale tri pa iz področja organske in anorganske kemije. Tudi za ta del imajo dijaki na voljo pet ur; naloge so zahtevne, zato dijake pripravljamo na Fakulteti za kemijo in kemijsko tehnologijo v Ljubljani.

Ves preostali čas dijakov na olimpijadi pa je namenjen druženju in spoznavanju države.

Letos je vsega skupaj tekmovalo 250 dijakov iz 64 držav. Vsako državo lahko zastopajo največ štirje dijaki in dva mentorja, ter seveda gostje. Na tej olimpijadi je zaradi bojazni pred prašičjo gripo, ki razsaja po Otoku, sodelovalo nekaj manj dijakov. Najboljši je bil dijak iz Kitajske, drugi je bil presenetljivo Izraelec, in tretji dijak iz Tajvana. Letos sta dva dijaka iz naše ekipe le za las zgrešila bronasto medaljo, in dobila posebno priznanje.

Naslednja olimpijada bo leta 2010 v Tokyu.

# POLETNA ŠOLA KEMIJE 2009

Na Fakulteti za kemijo in kemijsko tehnologijo smo tokrat drugič organizirali poletno šolo kemije. Vodja poletne šole je bil dr. Andrej Godec, pri organizaciji pa sta sodelovala še Zveza za tehniško kulturo Slovenije in Zavod RS za šolstvo.

Poletna šola je potekala v tednu od 29. 6. do 3. 7. 2009, v njej pa je sodelovalo 18 dijakov iz cele Slovenije.

Udeležence poletne šole smo v ponedeljek dopoldne sprejeli na FKKT. Navzoče je najprej pozdravil dr. Andrej Godec. V imenu gostitelja, Fakultete za kemijo in kemijsko tehnologijo, je navzoče nagovoril predsednik akademskega zbora fakultete prof. dr. Ciril Pohar.

Udeležencem pa sta želela uspešno delo v poletni šoli še gospod Rado Stojanovič v imenu ZOTKS in mag. Andreja Bačnik v imenu Zavoda RS za šolstvo.

Po otvoritvi in pogostitvi so dijaki najprej poslušali predavanje o kemijski varnosti z osnovami toksikologije (mag. Andreja Bačnik). Nato pa so pričeli z delom v laboratoriju katedre za analizno kemijo. Prvo delavnico je vodila dr. Helena Prosen, pomagala pa je tehnična sodelavka Mojca Žitko.

Na tej delavnici so se dijaki ukvarjali s trdoto vode. Poleg tega pa so s tekočinsko kromatografijo določali kofein v različnih pijačah.

Naslednji dan so dijaki preživeli dopoldne na fakulteti, popoldne pa na izletu z ladjico po Ljubljanici. Del tega je bil tudi krajši piknik na njenem bregu.

Tretji dan poletne šole je bilo na vrsti delo v laboratorijih katedre za organsko kemijo. To delavnico je vodil dr. Janez Cerkovnik, pomagala pa mu je Zdenka Kadunc.

Na tej delavnici so dijaki sintetizirali barvilo metiloranž, in testirali njegove indikatorske lastnosti. Razen tega pa so s pomočjo destilacije z vodno paro in ekstrakcije z diklorometanom izolirali eterična olja iz semen janeža, kumine in klinčkov ter lupin pomaranče in limone.

Četrti dan so dijaki preživeli v laboratorijih katedre za anorgansko kemijo. To delavnico sta vodili dr. Romana Cerc Korošec in dr. Elizabeta Tratar Pirc, pomagal pa jima je Damjan Erčulj.

Dijaki so sintetizirali bakrov hialuronat in ga okarakterizirali z nekaterimi osnovnimi kemijskimi metodami. Ugotavljali so še, pri katerih pogojih lahko hialuronatne raztopine gelirajo.

Druga skupina dijakov pa je pripravila tanke plasti titanovega dioksida po sol-gel postopku in jih s tehniko potapljanja nanašala na silicijeve rezine. Nato pa so ugotavljali še fotokatalitske sposobnosti te spojine.

Poletna šola je z aktivnostmi prenehala v petek, ko je bil na vrsti slovesen zaključek. Po uvodnem nagovoru so dijaki sami predstavili svoje delo v vseh delavnicah poletne šole. Zbrane je nagovoril tudi prodekan FKKT prof. dr. Anton Meden, ki je vsem skupaj zaželel veliko veselja s kemijo, in izrazil željo, da se še vidimo. Na koncu je dijakom razdelil še priznanja o udeležbi na poletni šoli kemije 2009.

Dijaki so nato izpolnili anketo o svojih vtisih. Iz odgovorov v anketah lahko sklepam, da je bila poletna šola 2009 uspešna, in da so dijaki na njej skozi delo na naši fakulteti spoznali nekaj novih in sodobnih kemijskih vsebin. Med njihovimi pripombami pa naj omenim željo po več stolih, kjer bi se lahko med delom v laboratoriju odpočili; enemu od njih pa se je zdela kemija precej »pocasta«.

Razšli smo se z željo, da se naslednje leto ponovno srečamo. Nasvidenje torej v poletni šoli kemije 2010!

Zahvala gre vsem sodelavcem naše fakultete, ki so pomagali pri izvedbi poletne šole, pa tudi obema partnerjema, ZOTKS in Zavodu RS za šolstvo, ki sta pomagala pri organizaciji.

## NOČ ZNANSTVENIC IN ZNANSTVENIKOV 2009

Direktorat za znanost in raziskave Evropske komisije je že skoraj tradicionalno (petič) organiziral in sofinanciral vseevropski znanstveni dogodek z naslovom »Noč znanstvenic in znanstvenikov 2009«. Namen teh dogodkov je bil predvsem ta, da bi širšo laično javnost na lahkoten, poučen in zabaven način seznanili z znanstvenimi dosežki. Seveda naj bi sam dogodek popestrili tudi s kemijskimi poskusi.

Dogodki naj bi bili take vrste, da bi bili zanimivi prav za vse – od otrok do starejših. In še več, dogodki naj bi bili predvsem neformalni, prijetni, sproščeni in privlačni.

Četudi EU posebej financira te dogodke, je UL FKKT izvedla svojo interno »Noč znanstvenic in znanstvenikov 2009«. Nekateri so to prireditev zaradi nekaterih nenavadnih poskusov že poimenovali »Noč čarovnic«, četudi terminsko ta dan ne ustreza. Pri izvedbi je sodelovala matična fakulteta, finančni del pa je pokrila raziskovalna programska skupina P1-0175LE. V veliki »novi predavalnici« fakultete smo izvedli vrsto kemijskih poskusov, uporabili pa tudi kemikalije, ki so splošno dostopne v gospodinjstvu. Pri izvedbi sva sodelovala naš vsestranski tehnični sodelavec g. Aleš Knez in prof. Ivan Leban. Bilo nam je prijetno – tako prireditelјem kot obiskovalcem je večer ostal v prijetnem spominu, četudi je bila na koncu le skromna zakuska. Mogoče nam je bilo v zadoščenje, da se je na spletni strani EU naš dogodek zapisal kot »Associated Event of Researchers Night 2009«.

Spletna računalniška predstavitev večera znanstvenikov 2009 je na spletni strani http://abra.fkkt.uni-lj.si/fn01leban/rn2009/ , temu zapisu pa je dodanih nekaj posnetkov s samega večera. Posebej so me razveselile radovedne oči naših otrok, pa tudi starejših. Nekateri najmlajši so z veseljem sodelovali tudi pri izvedbi poskusov. Na prireditvi je bilo skupaj preko 150 obiskovalcev. Zastopani so bili najmlajši, pa tudi starejših ni manjkalo. V septembru 2010 načrtujemo podobno prireditev z novo serijo kemijskih poskusov. Je pač že tako, da so poskusi v živo povsem drugačni kot oni, ki jih lahko najdete na virtualnem računalniškem spletu.

## SKRB FAKULTETE ZA VARSTVO OKOLJA – RAVNANJE Z ODPADKI

V skladu s Pravilnikom o ravnanju z odpadki (Ur l. RS št. 84/98 ter spremembe in dopolnitve pravilnika) na fakulteti ločeno zbiramo naslednje vrste odpadkov:

1. nevarne odpadke,
2. odpadne baterije,
3. ostali odpadki.

Nevarni odpadki in odpadne baterije se po pravilniku štejejo med posebne vrste odpadkov. Komunalni odpadki tukaj niso zajeti.

## 1. NEVARNI ODPADKI

Nevarni odpadek je odpadek, razvrščen v eno od skupin v klasifikacijskem seznamu nevarnih odpadkov, določenem v prilogi zgoraj navedenega pravilnika.

Laboratorijski red FKKT prepoveduje zlivanje nevarnih snovi v odtoke in odlaganje v smeti. Sistem zbiranja nevarnih odpadkov je bil na fakulteti postavljen 1. 3. 2000.

Zbirajo se naslednji nevarni odpadki: eksplozivni, oksidativni, lahko vnetljivi in vnetljivi, strupeni in jedki odpadki ter odpadna olja; ločeno po skupinah:

- halogenirana odpadna topila,
- nehalogenirana odpadna topila,
- odpadne tekoče anorganske kisline (pH < 2),
- odpadni tekoči lugi (pH > 11,5),
- odpadna olja,
- odpadni peroksidi,
- cianidi,
- odpadne neznane kemikalije.

Jedke kemikalije v območju pH od 2 do 11,5 se nevtralizira. pH vrednost razredčene kemikalije pred izpustom v kanalizacijo mora biti v območju od 5 do 9.

Za zbiranje nevarnih odpadkov so na razpolago ročke iz polietilena PE-HD, volumna 3, 5 in 10 L. Material PE-HD je ustrezen za shranjevanje večine odpadnih kemikalij, razen za halogenirana topila in močne oksidante (ti se zbirajo v njihovih praznih komercialnih embalažah, enako kot druge kemikalije, za katere PE-HD embalaža ni ustrezna).

Na embalažo za odpadne kemikalije se nalepi nalepka, na kateri se vpiše:

- klasifikacijska številka iz seznama nevarnih odpadkov,
- datum oddaje,
- katedra,
- podpis osebe, ki odda nevarni odpadek,
- ime oz. skupino kemikalije ter oznako nevarnosti za posebne odpadne kemikalije.

Odpadne kemikalije se zbirajo v kontejnerju za nevarne odpadke na dvorišču tehnične šole in predajo pooblaščenemu prevzemniku odpadkov. Za vsak odpadek se izpolni evidenčni list.

## 2. ODPADNE BATERIJE

Zbirajo se posebej in predajo pooblaščenemu prevzemniku odpadkov ter izpolni evidenčni list.

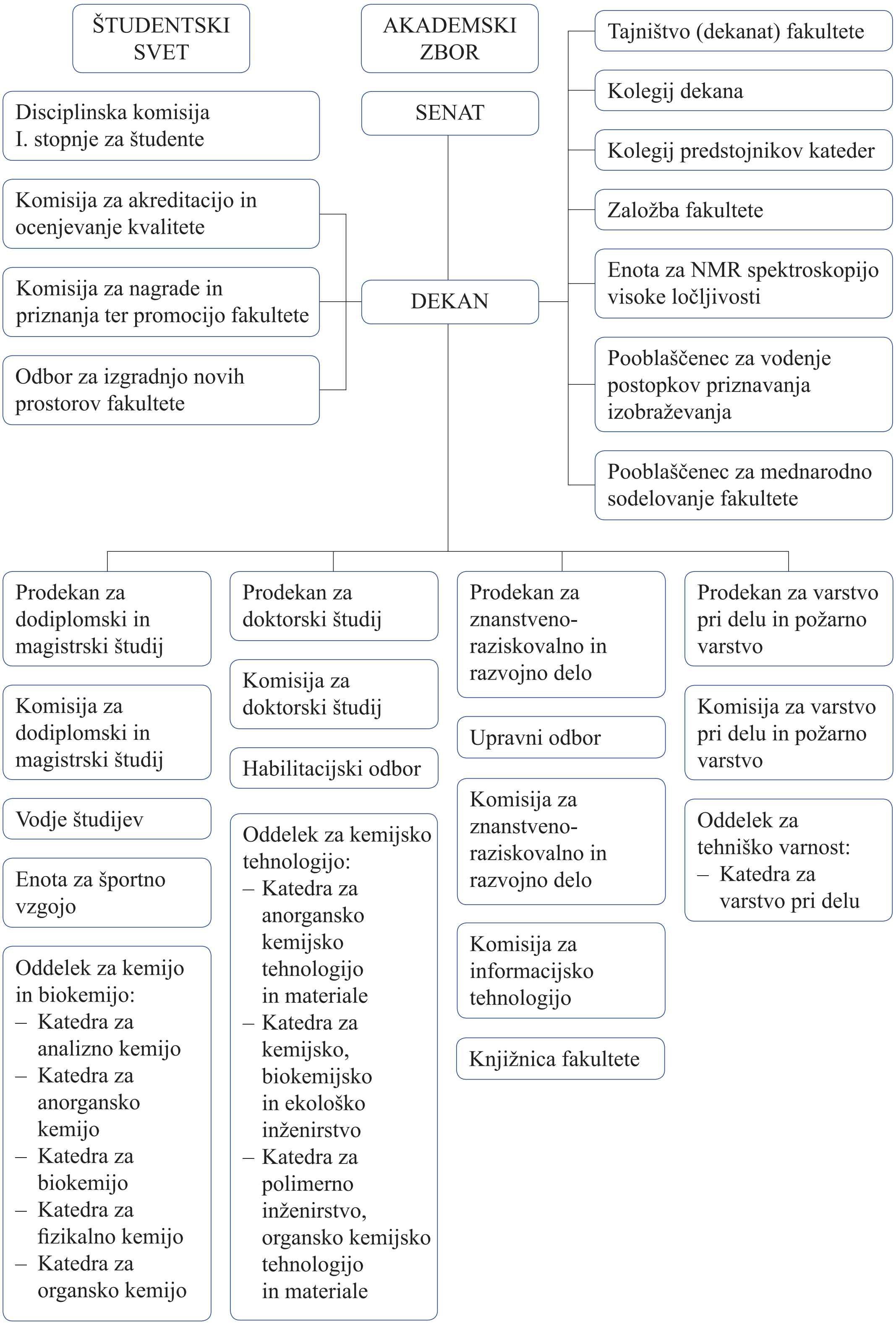
## 3. OSTALI ODPADKI

Ločeno se zbira še:

- prazne kartuše tiskalnikov
- električno in elektronsko opremo

in oddaja pooblaščenemu prevzemniku odpadkov. Za vsak odpadek se izpolni evidenčni list.

# ORGANIZACIJSKA SHEMA



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## DIPLOME

### UNIVERZITETNI ŠTUDIJSKI PROGRAMI

### KEMIJA

**Mateja Bartol**
Mentor: doc. dr. Andrej Pevec
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**Leon Bedrač**
Mentor: prof. dr. Marko Andrej Zupan
Somentor: dr. Jernej Iskra, viš. znan. sod.
Sinteza diklorojodatov (I) in njihova uporaba v reakcijah jodiranja
Datum zagovora: 7. 7. 2009

**Tjaša Berginc**
Mentorica: doc. dr. Romana Cerc Korošec
Somentorica: dr. Polona Umek, viš. znan. sodel.
Sinteza in karakterizacija nanodelcev $\alpha$-$MnO_2$ dopiranih z ioni $Fe^{3+}$, $Cr^{3+}$ in $Co^{2+}$
Datum zagovora: 23. 6. 2009

**Tadeja Birsa Čelič**
Mentorica: doc. dr. Amalija Golobič
Somentor: prof. dr. Venčeslav Kaučič
Sinteza in strukturna karakterizacija poroznih železovih karboksilatov
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**Tanja Bošković**
Mentor: prof. dr. Boris Pihlar
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Datum zagovora: 17. 9. 2009

**Lucija Brajer**
Mentor: doc. dr. Bojan Kozlevčar
Sinteza in karakterizacija koordinacijskih spojin z etilendiamintetraocetno kislino EDTA
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**Neja Brezavšček**
Mentor: doc. dr. Bogdan Štefane
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**Maja Brkić**
Mentor: prof. dr. Primož Šegedin
Sinteza in karakterizacija spojin kobaltovega(II) acetata s piridinom
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**Sašo Čebašek**
Mentor: prof. dr. Vojko Vlachy
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**Miha Friedrich**
Mentor: prof. dr. Jurij Svete
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**Ksenija Gačnik**
Mentorica: doc. dr. Amalija Golobič
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**Petra Galer**
Mentor: prof. dr. Boris Šket
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**Martin Gazvoda**
Mentor: prof. dr. Marijan Kočevar
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**Monika Janjić**
Mentor: prof. dr. Jurij Svete
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**Sonja Kiraly Potpara**
Mentor: prof. dr. Jurij Svete
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**Urška Kocjan**
Mentor: prof. dr. Albin Pintar
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**Nataša Kovačević**
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Somentorica: prof. dr. Ingrid Milošev
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**Anita Krančič**
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Somentor: doc. dr. Gregor Muri
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**Katja Kravanja**
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**Slavko Laljek**
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Somentor: prof. dr. Miran Gaberšček
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**Simona Lavrič**
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**Simona Lojevec**
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**Tomaž Lukanc**
Mentorica: doc. dr. Helena Prosen
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**Kostja Makarovič**
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**Snežana Marković**
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**Tina Marolt**
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**Eva Menart**
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**Mateja Mihelič**
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**Tilen Novšak**
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**Miha Pate**
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**Darja Pečko**
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**Mojca Pešak**
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**Simona Prelesnik**
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**Samo Smrke**
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**Katja Škof**
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**Katja Štajner**
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**Katija Štubljar**
Mentor: doc. dr. Bojan Kozlevčar
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**Erika Švara**
Mentor: prof. dr. Boris Pihlar
Somentor: prof. dr. Andraž Legat
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**Matej Vizovišek**
Mentor: prof. ddr. Boris Turk
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**Majda Zor**
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**Darja Žerovnik**
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## KEMIJSKO IZOBRAŽEVANJE

**Irena Šutar**
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**Kostja Makarovič**
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## BIOKEMIJA

**Renata Blatnik**
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**Matija Brecelj**
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**Miha Butinar**
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**Peter Cimermančič**
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**Jena Doležal**
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**Petra Furlani**
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**Urška Granda**
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Somentor: prof. dr. Ivan Kreft
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**Miha Jakovac**
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**Sabina Kastelic**
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**Marina Klemenčič**
Mentorica: prof. dr. Brigita Lenarčič
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**Jernej Kovač**
Mentor: doc. dr. Marko Dolinar
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**Martina Lenarčič**
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**Erika Lipovšek**
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Somentor: doc. dr. Tomaž Marš
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**Ajasja Ljubetič**
Mentor: prof. dr. Roman Jerala
Somentor: doc. dr. Janez Štrancar
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**Samanta Makovac**
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**Nina Mencin**
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**Andreja Mirtič**
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**Anita Mužerlin**
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**Metka Novak**
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**Andrej Ondračka**
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**Janez Orehek**
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**Edo Prašnikar**
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**Jelena Rajković**
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**Sabina Rojko**
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**Tjaša Stare**
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**Maja Stojanović**
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**Martin Štefanič**
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**Primož Treven**
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**Martin Turk**
Mentor: prof. dr. Robert Zorec
Somentor: prof. dr. Marko Kreft
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**Domen Zafred**
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**Urška Žvab**
Mentorica: doc. dr. Kristina Gruden
Priprava prebavnih peptidaz koloradskega hrošča – intestainov v *E. coli* po transkriptih iz na krompirjeve inhibitorje peptidaz prilagojenih prebavil koloradskega hrošča
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## KEMIJSKO INŽENIRSTVO

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Indukcija biosinteze esteraze na industrijskem gojišču
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Sinteza in karakterizacija cirkonijevega hidrazin karboksilata
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Razvoj postopka izolacije karboksilnih kislin iz bio-olja
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Sinteza in karakterizacija nanokompozitnih mikrosfernih akrilatnih lepil
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Vpliv nekovinskih vključkov na proizvodnjo jeklenih izdelkov s tehniko preciznega štancanja
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Vpliv procesnih parametrov na polimerizacijo polisiloksanov v emulziji
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Vpliv morfologije in velikosti delcev na elektrokemijske lastnosti litij železo silikatnega katodnega materiala.
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Vplivi procesnih parametrov kristalizacije na lastnosti učinkovine s hipertenzičnim delovanjem
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Vplivi priprave zmesi bitumnov in gumenega prahu na reološke in mehanske lastnosti zmesi
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**David Voglar**
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## VISOKOŠOLSKA ŠTUDIJSKA PROGRAMA

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**Goce Atanasov**
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Adsorpcija takrolimusa na različnih nosilcih
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Adsorpcija vankomicina na Amberlit XAD16 v ekspandiranem sloju
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Vpliv dodatka volumskih ekspanderjev na tokovne lastnosti krvi
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Vpliv hitrosti mešanja na mikrokapsulacijo parafinskega voska z melaminsko smolo
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Vpliv stopnje nenasičenosti in procesa sinteze nenasičenih poliestrskih smol na mehanske lastnosti utrjenih smol
Datum zagovora: 14. 9. 2009

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Mikrovalovna sinteza železovega silikalita-1
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Karakterizacija koloidnih sistemov z metodo sipanja svetlobe
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Kompleksi cinkovega in nikljevega klorida z O-donorskimi ligandi
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Mikrovalovno sušenje izolacijskih plošč na osnovi perlita
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Vpliv granulacije in oblike zrn kremenčevega peska na kakovost livarskih jeder
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Vpliv delovanja encimov na lastnosti vlaknin iz različnih vrst lesa
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**Alenka Sintič**
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Datum zagovora: 15. 12. 2009

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Datum zagovora: 16. 10. 2009

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Datum zagovora: 26. 3. 2009

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Datum zagovora: 15. 12. 2009

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Datum zagovora: 2. 2. 2009

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Primernost Sia metode za ocenjevanje požarne varnosti
Datum zagovora: 19. 11. 2009

**Maks Petek**
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Datum zagovora: 16. 4. 2009

**Bojan Petrič**
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Datum zagovora: 26. 2. 2009

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Hiše s pasivnim ogrevanjem
Datum zagovora: 28. 10. 2009

**Boštjan Polak**
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Datum zagovora: 5. 3. 2009

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**Bruno Rupnik**
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Datum zagovora: 5. 3. 2009

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Datum zagovora: 14. 7. 2009

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**Primož Strnad**
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Datum zagovora: 2. 2. 2009

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Vpliv industrije ter prevoza nevarnih snovi ob reki v zaščitenem področju
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Varna uporaba fitofarmacevtskih sredstev
Datum zagovora: 21. 12. 2009

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Požarnovarnostni ukrepi pri vzdrževalnih delih
Datum zagovora: 23. 6. 2009

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Motiviranost delavcev nasploh in posebej pri uporabi osebne varovalne opreme
Datum zagovora: 8. 12. 2009

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Varna uporaba fitofarmacevtskih sredstev v vinogradih
Datum zagovora: 23. 6. 2009

**Uroš Žibert**
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Vloga ograj in cestne infrastrukture pri varnosti voznikov enoslednih motornih vozil
Datum zagovora: 26. 2. 2009

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## KEMIJA

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Razvoj analizne metode za določevanje kloramfenikola v mleku in mlečnih izdelkih s tekočinsko kromatografijo z masno spektrometrijo
Datum zagovora: 19. 1. 2009

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Datum zagovora: 30. 6. 2009

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Datum zagovora: 23. 10. 2009

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Datum zagovora: 26. 3. 2009

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Vpliv reakcijskih pogojev na transformacije fenil substituiranih alkoholov, alkenov in ketonov z X-L reagenti
Datum zagovora: 27. 3. 2009

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Študij halogeniranja organskih molekul v vodi in fluoriranih topilih
Datum zagovora: 7. 4. 2009

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Raziskave reakcijskih pogojev za jodo- in fluorotransformacije organskih molekul
Datum zagovora: 7. 4. 2009

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Stabilnost in termodinamika vezanja proteinov udeleženih pri programirani celični smrti bakterij
Datum zagovora: 17. 4. 2009

**Simona Peterlin**
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Vrednotenje aktivne površine papirniških vlaken in njene vezivne sposobnosti z adsorpcijo barvil
Datum zagovora: 27. 5. 2009

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Polifunkcionalizirani poliedrični silseskvioksani kot modifikatorji površin kovin, tekstila in polimernih veziv
Datum zagovora: 12. 6. 2009

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Sinteza substituiranih diazenov in njihova uporaba kot reakcijskih intermediatov
Datum zagovora: 3. 7. 2009

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Somentor: prof. dr. Slovenko Polanc
Funkcionalizacije površin elektroaktivnih materialov z organskimi molekulami
Datum zagovora: 8. 7. 2009

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Mentorica: prof. dr. Monika Jenko
Somentor: prof. dr. Boris Pihlar
Mehanizem in kinetika nastanka in odstranjevanja visokotemperaturnih oksidnih plasti na površini FeCrNiMoN zlitin
Datum zagovora: 8. 7. 2009

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Mehanska in kemijska stabilnost kromatografskih metakrilatnih monolitov in njihova miniaturizacija
Datum zagovora: 7. 7. 2009

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Interakcije hidrotrioksidov in divodikovega trioksida z Lewisovimi bazami in kislinami
Datum zagovora: 19. 10. 2009

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Datum zagovora: 21. 10. 2009

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Analiza produktov pri simulaciji kajenja ilegalnega kokaina
Datum zagovora: 21. 10. 2009

**Vojmir Francetič**
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Vpliv samourejanja aluminijevih koordinacijskih spojin pri sol-gel pripravi $Al_2O_3$
Datum zagovora: 23. 10. 2009

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Določitev struktur oksidacijskih razpadnih produktov atorvastatina
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**mag. Andrej Kocijan**
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Razvoj analiznih metod za spremljanje biosinteze in kvalitete statinov
Datum zagovora: 27. 11. 2009

## KEMIJSKO INŽENIRSTVO

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Statistično modeliranje pri oceni požarnega tveganja
Datum zagovora: 15. 1. 2009

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Modeliranje odstranjevanja ogljikovih in dušikovih spojin z imobilizirano biokulturo
Datum zagovora: 3. 7. 2009

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Datum zagovora: 6. 7. 2009

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Razvoj tehnologij za pripravo zaščitnih filtrov po sol-gel postopkih
Datum zagovora: 7. 9. 2009

# RAZISKOVALNI PROGRAMI Z ZAČETKOM FINANCIRANJA V LETU 2009

## RESEARCH PROGRAMMES STARTING IN 2009

| **NOSILEC** / PRINCIPAL RESEARCHER | **NASLOV** / TITLE |
|---|---|
| Prof. dr. Peter Bukovec | Bioanorganska in bioorganska kemija<br>*Bioinorganic and bioorganic chemistry* |
| Prof. dr. Boris Pihlar | Raziskave in razvoj analiznih metod in postopkov<br>*Research and development of analytical methods and procedures* |
| Prof. dr. Ivan Leban | Sinteza, struktura, lastnosti snovi in materialov<br>*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<br>*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<br>*Physical chemistry* |
| Prof. dr. Marijan Kočevar | Organska kemija: sinteza, struktura, aplikacija<br>*Organic chemistry: synthesis, structure and application* |
| Izr. prof. dr. Matjaž Krajnc | Kemijsko inženirstvo<br>*Chemical engineering* |
| Prof. dr. Janvit Golob | Separacijski procesi toplogrednih plinov za trajnostni razvoj<br>*Separation processes of greenhouse gases for sustainable development* |
| Prof. dr. Dušan Turk* | Strukturna biologija<br>*Structural biology* |
| Prof. dr. Igor Križaj* | Toksini in biomembrane<br>*Toxins and biomembranes* |
| Izr. prof. ddr. Boris Turk* | Proteoliza in njena regulacija<br>*Proteolysis and its regulation* |
| Akad. prof. dr. Janez Levec** | Kemijsko reakcijsko inženirstvo<br>*Chemical reaction engineering* |
| Izr. prof. dr. Janez Plavec** | Kemija in struktura bioloških učinkovin<br>*Chemistry and structure of biologically active compounds* |
| Izr. prof. dr. Albin Pintar** | Integralni pristop k preprečevanju onesnaževanja voda<br>*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**

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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, kovinske spojine v okolju in njihova imobilizacija, razvoj novih sintetskih metod, študij mehanizmov bromiranja.

## OSREDNJE TEME PROGRAMA

Kemija molibdenovih klastrov, bioaktivni kompleksi, kovine v okolju, nanocevke, emulzije in zelena kemija, jodiranje z elementarnim jodom, novi organski peroksidi, nove metode bromiranja.

## ZNANSTVENI IN DRUGI RELEVANTNI DOSEŽKI

### BIOANORGANSKI SKLOP

V okviru raziskav koordinacijskih spojin molibdena(V) z večveznimi ligandi je bila podrobneje raziskana reakcija izhodne, enojedrne koordinacijske zvrsti molibdena $[MoOCl_4(H_2O)]^-$ s pirazinom. Pri različnih reakcijskih pogojih je bilo izoliranih več kompleksov: dvojedrna iona $[\{MoOCl_3(Pyz)\}_2O]^{2-}$ in $[(MoOCl_4)_2(Pyz)]^{2-}$ ter štirijedrni ion s sestavo $[(Mo_2O_4Cl_4)_2(Pyz)_2]^{4-}$. Kot je potrdila rentgenska strukturna analiza, je bila v slednjih dveh zvrsteh realizirana mostovna vezava dušikovega liganda. Pripravljene so bile tudi analogne spojine z bromidnimi ioni kot ligandi. Študije magnetne susceptibilnosti ionskih spojin, ki vsebujejo dvojedrne $[(MoOX_4)_2(Pyz)]^{2-}$ ($X = Cl, Br$) anione in tetraetilamonijeve ali tetrafenilfosfonijeve katione, potrjujejo vpliv kristalne strukture oz. pakiranja gradnikov v trdnem stanju na magnetne lastnosti spojin. Opisano študijo smo že objavili.

Fotokatalitsko aktivne tanke plasti $TiO_2$ smo pripravili po sol-gel postopku iz prekuzorja $TiCl_4$. Stabilen sol smo s tehniko potapljanja nanesli na podlago, sledila je toplotna obdelava na 700 ºC. Velikost delcev anataza v tanki plasti, ki je bila 30 minut izpostavljena tej temperaturi, doseže 30 nm. Ta plast je bila fotokatalitsko precej aktivna, saj se je modelna maščobna substanca metilstearat pod vplivom UVA svetlobe razgradila v manj kot 30 minutah, kar kaže na potencialno uporabnost pripravljene plasti za samočistilno površino.

Proučevali smo anaerobno razgradnjo glukoze v prisotnosti cianidov. Sestavo nastalega bioplina smo določali s plinsko kromatografijo sklopljeno z masno spektrometrijo. Centrifugatom pred in po anaerobni razgradnji smo določali kemijsko porabo po kisiku (KPK), proste cianide, amoniak in hlapne maščobne kisline.

Naslednje raziskovalno področje pa je bilo usmerjeno v pripravo in proučevanje nano-MgO nanesenega na različne nosilce ($\gamma$-$Al_2O_3$ prah, steklo, molekularna sita) ter ugotavljanje protimikrobne aktivnosti pripravljenih materialov. Proučevali smo tudi protimikrobne aktivnosti nano srebra nanesenega na hialuronatne filme, pripravljenih po različnih sinteznih postopkih.

Nadaljevali smo z raziskovanjem $CeO_2$ ionskih hranilnikov, pripravljenih iz anorganskih prekurzorjev po sol-gel postopku. Pri pripravi mešanih oksidov cerija in vanadija z množinskim razmerjem 1:1 smo kot topilo uporabili metanol oz. destilirano vodo. Elektrokemijske, optične in strukturne lastnosti tankih plasti smo raziskovali s termično analizo, ciklovoltametrijo (CV), kronokulometrijo (CPC) in različnimi optičnimi metodami. V sodelovanju z Univerzo v Mariboru smo izvedli meritve podaljšane fine strukture rentgenskih robov (EXAFS).

Na področju kemijske stabilizacije kovin v onesnaženih tleh smo izvedli obširno raziskavo na umetno onesnaženih tleh, katerih koncentracije kovin so dosegale povprečne vrednosti, ki so jih našli v Mežici. Proučevali smo mobilnost kovin v tleh ter izvedli njihovo stabilizacijo z različnimi dodatki. Z izluževalnimi kolonskimi testi smo simulirali padavine kot izluževalni medij, ter tako ovrednotili dolgoročno uspešnost stabilizacije. Delne rezultate raziskav smo predstavili na Slovenskih kemijskih dnevih 2009 in na mednarodni konferenci CEST 2009 na Kreti.

Kurkumin (1,7-bis(4-hidroksi-3-metoksifenil)hepta-1,6-dien-3,5-dion) je zaradi fenolnih hidroksilnih skupin močan antioksidant. Literaturni podatki kažejo na to, da je kurkumin naravni inhibitor transkripcijskega faktorja NF-κB in zaradi tega zanimiv za raziskovanje njegovega vpliva na zmanjšanje rezistentnosti tumorskih celic na citostatike. Z vidika ohranitve antioksidativnih lastnosti kurkumina smo se odločili tudi za pripravo derivata kurkumina s prostima fenolnima hidroksilnima skupinama in substituentoma na mestu -OMe skupin, ki imajo afiniteto do vezave na Pt(II) ion. V letu 2009 smo poskusili sintetizirati 3-amino-4-hidroksibenzaldehid in njegov *N*-acetil derivat. Za izboljšanje izkoristka smo preučevali različne načine redukcije s Sn, $SnCl_2$, Zn, $H_2$/Pd in $Na_2S$. Zaradi slabe perspektive pri sintezi amino derivata vanilina smo preusmerili prizadevanja na pripravo aminokislinskega derivata vanilina. Citotoksično aktivnost novih Pt(II) spojin v primerjavi s cisplatinom smo v sodelovanju z Onkološkim inštitutom v Ljubljani tudi testirali.

## BIOORGANSKI SKLOP

Preučevali smo vpliv joda kot katalizatorja organskih transformacij. Ugotovili smo, da učinkovito katalizira prenos acetilne skupine pod reakcijskimi pogoji brez topila. Fenil-substituirani aldehidi se pri tem pretvorijo v ustrezne 1,1-diacetate, alkoholi pa v acetatne estre. Pokazali smo, da je vrstni red dodajanja reaktantov ključnega pomena za potek transformacije; v primeru kompleksacije joda reakcija ne poteče. Acetanhidrid je najboljši prenosnik acetilne skupine, izopropenil acetat in vinil acetat sta manj učinkovita. Nadalje smo ugotovili, da jod katalizira estrenje alkoholov pod reakcijskimi pogoji brez topila – opazili smo dvojno obnašanje alkoholov. Estrenje alkilnih alkoholov poteče z ohranitvijo absolutne konfiguracije, medtem ko iz benzilnih alkoholov dobimo optično neaktivne estre. Tak potek pripisujemo stabilnosti karbokationa, ki nastane iz alkohola. Ugotovili smo, da je estrenje kot reverzibilna reakcija presenetljivo malo občutljiva na prisotnost vode; voda ki nastaja pri reakciji ne pomakne ravnotežja v smer reaktantov. Reaktivnost alkilnih karboksilnih kislin pada z naraščajočo razvejanostjo in dolžino verige.

Študirali smo transformacije alkil-substituiranih benzenov z *N*-bromosukcinimidom pod vplivom vidne svetlobe (volfram, 40 W) pod reakcijskimi pogoji brez topila. Ugotovili smo, da pri teh pogojih poteče Wohl-Zieglerjeva reakcija, produkti so benzil bromidi. Elektron-privlačne skupine na aromatskem jedru zmanjšajo reaktivnost substratov. Iz anizola nastane 4-bromoanizol, iz acetofenona pa zmes α-bromo in α,α-dibromo ketona.

V okviru laboratorija za organsko in bioorgansko kemijo smo nadaljevali raziskave na področju transformacij, s poudarkom na halogeniranju organskih spojin pod okolju prijaznejšimi reakcijskimi pogoji. Razvili smo selektivno in učinkovito metodo za direktno fluoriranje ketonov v vodnem mediju z reagentom *Selectfluor*$^{TM}$ F-TEDA-$BF_4$ ob prisotnosti anionskega surfaktanta natrijevega dodecil sulfata v količini nad njegovo kritično micelno koncentracijo. Proučili smo tudi transformacije organskih spojin z F-TEDA-$BF_4$ v ionskih tekočinah kot reakcijskem mediju. Sintetizirali smo vrsto alkil in aril jod(III) dikloridov, ki vsebujejo perfluoroalkilne verige, proučili njihove lastnosti in reaktivnost ter na osnovi tega razvili metodo za kloriranje organskih spojin, ki vključuje regeneracijo reagenta kot perfluoro substituiranega jodida, njegovo ponovno kloriranje s $Cl_2$ in nadaljnjo uporabo v procesu kloriranja organskih spojin. Razvili smo okolju prijazno metodo za elektrofilno in radikalsko bromiranje organskih spojin v vodnem mediju z uporabo reakcijskega sistema $HBr/H_2O_2$ ali N-bromsukcinimida. Prvi reagent se je pokazal za učinkovitejšega za bromiranje ketonov in benzilno derivatizacijo, medtem ko je drugi učinkovitejši za bromiranje aktiviranih aromatov. Razvili smo okolju prijazno metodo za dibromiranje alkenov po načinu aerobnega oksidativnega bromiranja z 48 % vodnim HBr in $NaNO_2$ kot katalizatorjem. Proučili smo tudi možnost benzilnega bromiranja alkil aromatov z N-bromsukcinimidom pod pogoji brez uporabe topila in ugotovili, da je taka transformacija zelo uspešna po aktivaciji sistema z vidno svetlobo moči 40 W. Prvim na svetu nam je uspelo razviti neencimatsko metodo aerobnega oksidativnega halogeniranja organskih molekul v vodnem mediju. Ketone smo selektivno in učinkovito jodirali v vodnem mediju z uporabo elementarnega joda, zraka kot oksidanta, $NaNO_2$ kot katalizatorja in $H_2SO_4$ kot aktivatorja celotnega katalitskega sistema. Dosegli smo popolno atomsko ekonomijo joda in ugotovili, da so procesi jodiranja učinkovitejši in hitrejši ob prisotnosti natrijevega dodecil sulfata v količini nad njegovo kritično micelno koncentracijo. Na povabilo uredništev smo pripravili pregledne članke ali poglavja v knjigah o halogeniranju organskih spojin v ionskih tekočinah, halogeniranju organskih spojin pod reakcijskimi pogoji brez uporabe topil, metodah oksidativnega halogeniranja organskih spojin z uporabo kisika ali vodikovega peroksida, okolju prijaznih metodah benzilnega bromiranja in o antibakterijskih organskih peroksidih. V sodelovanju s podjetjem Krka d.d. smo razvili neodvisni postopek za pripravo antibiotske učinkovine kinolonskega tipa.

## RESEARCH PROGRAMME REPORT

### PROGRAMME GOALS

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

### RESEARCH TOPICS

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

### SCIENTIFIC AND OTHER RELEVANT ACHIEVEMENTS

#### BIOINORGANIC CHEMISTRY

In continuation of our ongoing research on molybdenum(V) coordination compounds with multidentate ligands, we have recently focused on the reaction of mononuclear $[MoOCl_4(H_2O)]^-$ ion with pyrazine. Small changes in the reaction conditions provided the following novel complexes: dinuclear anions $[\{MoOCl_3(Pyz)\}_2O]^{2-}$ and $[(MoOCl_4)_2(Pyz)]^{2-}$, and tetranuclear anion $[(Mo_2O_4Cl_4)_2(Pyz)_2]^{4-}$. In the last two species, the X-ray structure analysis has confirmed a bridging role of the nitrogen donor ligand. Similar reactions with the bromide starting material resulted in analogous bromido complexes. Temperature dependent studies of magnetic susceptibility of dinuclear $[(MoOX_4)_2(Pyz)]^{2-}$ (X = Cl, Br) compounds have revealed indirect influence of the nature of countercations upon the magnetic properties. The study has just been published.

Photocatalitically active thin films of titania were prepared by sol-gel method using $TiCl_4$ as a precursor. The stable sol was deposited on a substrate by dip-coating technique, and then thermally treated at 700 ºC. The size of the anatase crystallites in the film, which was treated for 30 minutes at 700 ºC, reached 30 nm. This film was photocatalitically very active. A model fatty contaminant methyl-stearate decomposed in less than 30 minutes after UVA illumination, showing a potential application of the prepared film as a self-cleaning surface.

Influence of cyanide on anaerobic degradation of glucose was investigated. Biogas composition was determined using gas chromatography coupled by mass spectrometry (GC/MS). We analysed centrifugates before and after anaerobic degradation (chemical oxygen demand (COD), free cyanides, ammonia and volatile fatty acids (VFA).

The main focus of another research area was the preparation and characterization of nano-MgO deposited on different substrates ($\gamma$-$Al_2O_3$ powder, glass, molecular sieves) and investigation of antibactericidal activities of prepared materials. Antibactericidal activity of nano-silver integrated into hyaluronate network prepared on different pathways was also investigated.

We also continued studies on $CeO_2$ ion-storage films prepared by sol-gel method from inorganic precursors. Mixed oxides thin films of cerium and vanadium were prepared at molar ratio 1:1 using methanol or distilled water as a solvent. The electrochemical optical and structural properties of thin films were investigated by thermal analysis, cyclovoltammetry (CV), chronocoulometry (CPC) and different optical methods. In collaboration with the Faculty of Mechanical Engineering in Maribor measurements of Extended X-ray Absorption Fine Structure (EXAFS) of the prepared thin films were performed.

In our research on chemical stabilization of metals in contaminated soil, an extensive study was performed with artificially contaminated soil with metal concentrations comparable with average soil metal concentrations reported for Mežica. The study involved determination of mobility of metals, investigation of their stabilization with addition of different stabilization agents and evaluation of long term stabilisation efficiency using column leaching tests as simulation of precipitations. Partial results of our study were presented at the 15th Slovenian Chemical Event 2009 and on 11th International Conference on Environmental Science and Technology, Crete, 2009.

Curcumin (1,7-bis(4-hydroxy-3-methoxy-phenyl)hepta-1,6-diene-3,5-dione) has a high antioxidative potential due to its phenol hydroxide groups. Literature survey indicates its natural transcription factor NF-κB inhibition property which makes it an interesting candidate for research of its influence on the resistance of tumor cells to cytostatic drugs. In order to preserve its antioxidative properties we decided to prepare a curcumin derivative with two free phenol hydroxide groups and two substitutes at the O-Me sites, having affinity to Pt(II) binding. In 2009 we attempted to synthesize 3-amino-4-hydroxybenzaldehyde and its *N*- acetyl derivative. To improve the procedure we studied several reduction options with Sn, $SnCl_2$, Zn, $H_2$/Pd and $Na_2S$. Due to obviously limited success in amino derivative of vanillin synthesis, an alternative synthesis of vanillin analogue with amino acid moiety was studied. Cytotoxic potential of the new Pt(II) compounds compared to cisplatin was assessed in collaboration with the Institute of Oncology, Ljubljana.

## BIOORGANIC CHEMISTRY

We were studying the effect of iodine as a catalyst in organic reactions. It was established that iodine effectively catalyzed the acetyl transfer under solvent-free reaction conditions. Phenyl-substituted aldehydes were converted to the corresponding 1,1-diacetate derivatives; alcohols were transformed to acetates. It was shown that the order of addition of the reactants was crucial for the reaction progress; in the case of complexation of iodine the reaction did not take place. Acetic anhydride was the most efficient acetyl transfer agent, while isopropenyl acetate and vinyl acetate were less effective. Further on we found iodine as an effective catalyst for the esterification of alcohols under solvent-free reaction conditions; the dual behaviour of alcohols was established. Esterification of the alkyl alcohols took place with the retention of absolute configuration, while benzylic alcohols furnished optically inactive esters. This could be attributed to the stability of the carbocation formed from alcohol. It was established that esterification as a reversible reaction exhibited surprisingly little sensitivity on the presence of water; the water released during the reaction did not shift the equilibrium to the direction of the reactants. The reactivity of the alkyl carboxylic acids decreased with the increasing branching and length of the chain.

Visible-light (tungsten, 40W) transformation of alkyl-substituted benzenes with *N*-bromosuccinimide under solvent-free reaction conditions was studied. Wohl-Ziegler reaction took place yielding benzyl bromides. Electron-withdrawing groups on the aromatic ring decreased the reactivity of the substrates. Anisol yielded 4-bromoanisole, acetophenone produced a mixture of α-bromo in α,α-dibromo ketone.

Within the framework of Laboratory for organic and bioorganic chemistry we continued the investigation on the application of principles of green chemistry to the transformations of organic compounds stressing the selective introduction of halogen atoms into organic compounds. We developed a selective and effective method for direct fluorination of ketones in aqueous media using the Selectfluor$^{TM}$ F-TEDA-$BF_4$ reagent in the presence of anionic surfactant sodium dodecylsulfate in the amounts above its critical micelle concentration. We have further investigated transformation of organic compounds with Selectfluor$^{TM}$ F-TEDA-$BF_4$ in ionic liquids as a reaction media. We have prepared a variety of fluorous and nonfluorous aryl and alkyl iodine(III) dichlorides, investigated their characteristics and reactivities and on this basis developed the method for chlorination of organic compounds which includes the protocol for regeneration of the reagent as fluorous iodides, its re-chlorination with $Cl_2$ and its further use in the chlorination process. We have developed an environmentally friendly method for electrophilic and radical bromination of organic compounds in aqueous media using $HBr/H_2O_2$ reaction system or – bromosuccinimide and compared their efficiency. The first reaction system has been found to be more efficient for the bromination of ketones and derivatisation of benzylic position, while NBS have been more efficient for the bromination of activated aromatics. Aerobic oxidative dibromination of alkenes was developed using 45% aqueous HBr and $NaNO_2$ as the catalyst. We have investigated a benzylic bromination of alkylaromatics with NBS under solvent-free reaction conditions and established that this transformation was promoted by 40W visible light irradiation. We introduced the first example of non-enzymatic aerobic oxidative halogenation of organic compound in an aqueous media. Ketones were selectively and efficiently iodinated in aqueous media using elemental iodine, air oxygen as terminal oxidant, $NaNO_2$ as the catalyst, and sulphuric acid as the activator of the overall catalytic system. The total iodine atom economy was accomplished while the process has been established to be more efficient and faster in the presence of anionic surfactant sodium dodecylsulphate in the amounts above its critical micelle concentration. On the basis of invitations we prepared review articles and chapters in books reviewing the halogenation of organic compounds in ionic liquids, the halogenation of organic compounds under solvent-free reaction conditions, methods for green oxidative halogenation of organic compounds using oxygen or hydrogen peroxide, green methods for benzylic bromination, and antibacterial organic peroxides. In collaboration with the pharmaceutical company Krka we have developed an independent protocol for the synthesis of precursors for quinolone-type antibiotics.

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

**PROGRAMSKA SKUPINA** / RESEARCH PROGRAMME GROUP

**P1–0153**

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# 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 2009 objavili 21 izvirnih znanstvenih člankov (bibliografija Katedre za analizno kemijo, *AL1-21*), en pregledni članek (*AL22*), dvoje vabljenih predavanj (*AL23-24*), 6 znanstvenih prispevkov na konferencah (*AL25-30*), tri samostojne znanstvene sestavke v znanstveni monografiji (*AL31-33*), o rezultatih pa so poročali tudi na večjem številu znanstvenih simpozijev in konferenc.

Raziskovali smo naslednje:

**a)**

Razvili smo metodo osnovano na povezavi masnega spektrometra pripojenih ionov (ion attachment MS, IAMS) v povezavi z infrardečo pečico, ki smo jo uporabili za pirolizo vzorcev. Opisana je primerjava s konvencionalno pirolizo GC/MS. Podan je tudi primer pirolize politetrafluoroetilena, pri katerem opazimo konstantno naraščanje intenzitete signala v odvisnosti od temperature v določenem temperaturnem območju. Za določen ion lahko tako določimo navidezno aktivacijsko energijo. Članek je bil objavljen v ugledni reviji *Analytical Chemistry* (*AL3*)

V članku objavljenem v *Journal of Physical Chemistry A* (*AL14*), smo z DFT izračuni z Gaussian programom optimizirali najnižje energije struktur fulerena in njegovih protoniranih oblik. Tako smo lahko izračunali protonsko afiniteto fulerena, ki je bila doslej le okvirno določena z eksperimentom, med 204 in 207 kcal/mol. Dobljena protonska afiniteta je bila 201,8 kcal/mol, kar se dobro sklada z eksperimentom. Določili smo tudi vseh pet prehodnih stanj in izračunali aktivacijske energije (*E*a), ki so bile med 27 in 90 kcal/mol.

Članek objavljen v *Analytical Chemistry,* z naslovom »Material degradomics: on the smell of old books« (*AL4*) obravnava nov inovativen pristop, ki smo ga poimenovali degradomika in je primeren za študij razgradnje materialov, še posebej papirjev zgodovinskega pomena. Osnova študije so bile hlapne spojine, ki izhajajo iz papirja. Njihova prisotnost in vsebnost je bila s pomočjo multivariantne analize korelirana z vsebnostjo najpomembnejših komponent papirja (kot so smole, lignin, karbonilne skupine, stopnja polimerizacije celuloze, kislost papirja), ki so pomemben pokazatelj lastnosti in stanja historičnih papirjev. Na podlagi profila hlapnih razgradnih produktov smo določili markerje, ki so povezani z vsebnostjo smol, lignina in preučevali njihov vpliv na razgradnjo papirja. Poleg ocetne kisline in furfurala, ki sta znana pokazatelja razgradnje, smo določili številne druge spojine, ki so produkti maščobne peroksidacije. Z določanjem hlapnih spojin, ki izhajajo iz papirja lahko na nedestruktiven način in hitro identificiramo uničene oziroma ogrožene zgodovinske objekte.

V članku objavljenem v ugledni reviji *Journal of Electrochemical Society* (*AL15*), smo opisali raziskavo mehanizma raztapljanja bakra v močno amoniakalnem mediju. Ugotovili smo, da na korozijo bakra v amoniakalnih raztopinah vplivajo različni dejavniki, predvsem koncentracija amoniaka, pH, temperatura, koncentracija $Cu^{2+}$, prisotnost/odsotnost raztopljenega kisika, sam kemizem in koncentracija anionov, koncentracija vmesnih produktov, še posebej $Cu^+$ adsorbiranih intermediatov in tvorbe oksidnega filma, kar ima za posledico pasivizacijo materiala. V tej študiji smo raziskovali korozijo bakra v širokem območju potenciala (od –1,4 V do 0 V vs. MSE) in v širokem razponu koncentracij različnih zvrsti (0,2–3,5 mol/L $NH_3$, 0–0,1 mol/L $Cu^{2+}$, pH 10–12,5). Za voltametrični odziv med –1,0 V in –0,6 V vs. MSE smo ugotovili, da je reakcija glede na amoniak drugega reda. Z uporabo elektrokemijskih in optičnih metod (SEM) smo ugotovili, da je najverjetnejši mehanizem pasivizacije dvostopenjski proces (elektrokemijski-kemijski) tvorbe $Cu_2O$. To domnevo smo potrdili z impedančno analizo pri različnih eksperimentalnih pogojih.

Vpliv različnih elektrodnih materialov na odziv amperometričnega biosenzorja za glukozo smo opisali v članku objavljenem v reviji *Electroanalysis* (*AL20*). Raziskava je predmet magistrskega dela in je bila izvedena v sodelovanju z raziskovalci KI. Raziskali smo različne elektrodne podlage kot je steklasti ogljik (GC), ogljikova vlakna (CF) in tiskane ogljikove electrode (SPC), različnih velikosti in geometrij. Senzor je bil osnovan na Ru-heksacianoferatu kot mediatorju za redukcijo peroksida z glukoza oksidazo, imobilizirano na polimerni polifenilendiaminski membrani. Pokazalo se je, da GC in SPC electrode kažejo značilen encimsko kataliziran odziv, medtem ko CF mikroelektrode kažejo linearni difuzijsko kontroliran odziv.

Članek objavljen v reviji *Int. J. Mass Spectrometry* (*AL11*), obsega razvoj metode za merjenje izotopskega razmerja plutonijevih radionuklidov na pikogramskem nivoju. Metoda je osnovana na masni spektrometriji s termično ionizacijo (TIMS), kjer smo optimizirali tehniko pirolitske priprave Re kolektorske nitke. Z variiranjem parametrov kot so parcialni tlak benzena ter tok in čas trajajna pirolize, smo dosegli optimalno sorpcijsko kapaciteto. Razvili smo tudi dinamično tehniko merjenja Pu izotopov s t.i. večkratnim ionskim štetjem (MIC), rezultate pa preverili z NBL-137 izotopskim standardom in medlaboratorijskimi primerjavami na ppt nivoju. Nov pristop bistveno izboljšuje točnost izotopskih analiz v okoljskih vrorcih in s tem možnosti za boljše sledenje porekla Pu izotopov v naravi.

S kombinacijo HPLC-MS smo študirali stabilnost statinov, ki se uporabljajo kot farmacevtska učinkovina za znižanje holesterola. Kot je to opisano v članku objavljenem v reviji *Environ. Chem. Lett*. (*AL9*), smo raziskovali njihovo stabilnost v različnih pogojih pri različnih pH, v različnih topilih in stabilnost pri obsevanju z UV oziroma vidno svetlobo. Dobljeni rezultati kažejo na močno odvisnost stabilnosti statinov v odvisnosti od pH, relativno stabilnost statinov pri obsevanju z vidno svetlobo in njihovo razgradnjo pri obsevanju z UV svetlobo, kar smo razložili z vzbujanjem elektronov v p–p* pas. V pri nizkih vrednostih pH smo opazili manjšo pretvorbo iz laktonske v hidroksi kislinsko obliko, kot pri enakem pH in obsevanju z vidno svetlobo. Daljša izpostavljenost obsevanju vodi k procesom razgradnje statinov. Pretvorba statinov je manjša v vodi kot v acetonitrilu.

Monolitni diski (CIM) predstavljajo številne možnosti za hitre in učinkovite separacije makromolekul. V sodelovanju s slovenskim proizvajalcem CIM diskov podjetjem BIA Separations, Ljubljana, je bil razvit nov CIM monolitni separacijski medij s hidrazidnimi funkcionalnimi (HZ) skupinami za specifično vezavo in imobilizacijo protiteles. To je bilo doseženo s kovalentno vezavo dihidrazida adipinske kisline na polimerni epoksi monolit, na katerega smo uspešno vezali dvoje protiteles. Kolone so pokazale dobro selektivnost, izmerjena pa je bila tudi dinamična vezavna kapaciteta diskov v analitski in preparativni zvedbi. Članek je bil objavljen v ugledni reviji *Journal of Chromatography* A (*AL12*).

V človeškem serumu predstavljata albumin (HSA) in immunoglobulin G (IgG), več kot 75 % vseh proteinov v plazmi. Le-ti onemogočajo detekcijo tistih, ki so v manjših koncentracijah in lahko predstavljajo markerje za različna bolezenska stanja. Delna odstranitev HAS in IgG je zato za analizo proteoma velikega pomena. V članku opisujemo optimizacijo pogojev za selektivno odstranitev HSA in IgG z afinitetno in psevdo-afinitetno kromatografijo z BIA Separations CIM Protein G diskom in Mimetic Blue SA A6XL stacionarno fazo za odstranitev HSA. Pufrsko raztopino za pospešitev vezave in elucije za CIM Proteing G disk, smo izbrali na podlagi oblike vrha in določili kapaciteto vezave. Ta je odvisna of pufrnega sistema in neodvisna od pretoka in koncentracije IgG. Uporabo kolone Mimetic Blue SA A6XL, smo okarakterizirali z uporabo človeške plazme. Selektivnost odstranitve je bila odvisna od količine plazme na koloni. Po končani optimizaciji smo kombinacijo obeh kolon uporabili za hkratno odstranitev obeh proteinov, IgG in HSA. Dosežke opisuje članek objavljen v *Journal of Chromatography A* (*AL13*).

Vpliv negotovosti osnovnih sestavin in nečistoč v kalibracijskih standardnih raztopinah opisuje članek, objavljen v reviji *Analytica Chimica Acta* (*AL2*). Da bi prepoznali glavne prispevke h kombinirani negotovosti, smo izpeljali splošno metodologijo za podrobno bilanco negotovosti za vsak posamezen ion v osnovnih zmesnih standardih, katerih koncentracije so se razlikovale do pet velikostnih redov. Potrdili smo, da je utemeljeno upoštevati masne deleže nečistoč v drugih kemikalijah, ko računamo masne koncentracije ionov v kombiniranih standardih in da je pri mnogih ionih to glavni vir negotovosti.

**b)**

Zgodovinski pergamenti so zelo kompleksen makromolekulski material. K temu precej prispeva različen naraven izvor, nehomogenost strukture kože, neznano okolje hrambe in potencialna lokalizirana razgradnja. Večina dosedanjih raziskav se je osredotočala na termične in strukturne analizne metode. Z analizo atmosfere, ki obdaja pergament med oksidacijo, smo dokazali da se tvorijo hlapni aldehidi, ki so lahko produkti razgradnje maščob. Oksidirane pergamente smo dodatno preučevali s kemoluminescenco in na ta način določili stopnjo oksidacije različno razmaščenih pergamentov. V članku »Autoxidation of lipids in parchment« objavljenem v reviji *Polymer Degradation and Stability* (*AL16*), smo dokazali, da sta nastanek peroksidov in količina emitiranih aldehidov povezana z vsebnostjo maščob v pergamentu. Na podlagi tega lahko zaključimo, da prisotnost lipidov lahko vodi do oksidativne razgradnje kolagena. Hkrati pa nam nedestruktivna metoda določanja hlapnih aldehidov omogoča oceniti stabilnost pergamentov.

V študiji kataliziranega utekočinjenja v prisotnosti etilen glikola, p-toluen sulfonske kisline ali žveplove(VI) kisline kot katalizatorjev, smo uporabili mikrokristalinično celulozo, Whatman filtrni papir št. 1, ter bombažni linters z molskimi masami 76.000, 699.000 in 1.910.000 g/mol. Proces smo spremljali gravimetrično, z uporabo rentgenske difrakcije preostale celuloze in s spremljanjem molske mase celuloze z uporabo velikostne izključitvene kromatografije. Neurejeni deli makromolekul so se razgradili že v začetni minuti procesa utekočinjenja. Kristalinični deli so sorazmerno stabilni tudi po daljših časih reakcije. Izsledki teh raziskav so objavljeni v reviji *Cellulose* (*AL7*).

Dupleksna nerjavna jekla sodijo zaradi svojih mehanskih in kemijskih lastnosti med strateško pomembne materiale. V sodelovanju z IMT in deloma jeklarno Acroni, je bila izvedena raziskava mehanizma in kinetike nastanka oksidnih plasti na površini FeCrNiMoN zlitin. Problematika dekapiranja in pasivacije dvofaznih zlitin, predvsem porazdelitve faz avstenita in ferita na ali tik ob površini, je pri nas in v svetu zelo aktualna. V raziskavi objavljeni v reviji *Applied Surface Science* (*AL5*), so bili vzorci izpostavljeni kisiku v visokem vakuumu, nastale tanke oksidne plasti pa raziskane z XPS v različnih globinah. Pokazalo se je, da oksidne plasti vsebujejo različne koncentracije kromovih oksidov, ki se zvišujejo v smeri proti notranjosti materiala, medtem ko se delež Fe-oksidov povečuje proti površini.

Oksidacija dupleksnih jekel oznake 2205 s kisikom v induktivno sklopljeni plazmi, je bila raziskana s pomočjo rentgenske fotoelektronske spektroskopije (XPS) in elektronske mikroskopije (SEM). Eksperimenti so bili izvedeni v širokem temperaturnem obsegu od sobne temperature pa vse do 700 ºC. Sestav nastalih tankih oksidnih plasti je bil analiziran z XPS, morfologija plasti pa raziskana s SEM pri povečavah vse do 10.000. Rezultati analiz so omogočili vpogled v sestavo Fe/Cr/Mn oksidnih plasti, ugotovljena pa je bila tudi korelacija s temperaturo. Rezultati teh raziskav so opisani v članku objavljenam v reviji *Corrosion Science* (*AL8*), tematika pa je tudi predmet doktorske disertacije (COBISS.SI-ID 30608133).

V okviru karakterizacije materialov smo se ukvarjali tudi z utekočinjanjem ostankov lesa. Utekočinjeni les smo poskušali uporabiti kot naravni zaščitni premaz. V okviru te raziskave smo določali stranske produkte predvsem levulinsko kislino, ki nastaja pri utekočinjanju lesa. Ti produkti bi lahko bili uporabni in bi tako zvečali ekonomičnost utekočinjanja. Rezultati teh raziskav so opisani v članku *Bioresource Technology* (*AL6*).

**c)**

Pregledni članek objavljen v reviji *International Journal of Molecular Sciences* (*AL22*), obsega pregled metod za analizo in pripravo vzorca za določitev najbolj pogostih mikotoksinov v različnih prehranskih vzorcih, ki so bile objavljene v zadnjem desetletju. Posebna pozornost je namenjena tekočinski kromatografiji s fluorecsentno in masnospektrometrično detekcijo, med tehnikami za pripravo vzorca pa so obravnavane predvsem različne ekstrakcije na trdno fazo. Prav tako je podan pregled redkeje uporabljanih metod analize in priprave vzorca. Obravnavani so tudi različni matriksi, kjer se določajo mikotoksini, tudi s stališča specifičnih lastnosti, ki so pomembne za analizo (hrana in pijača, krma, biološki in okoljski vzorci). Kritično so obravnavani tudi različni vidiki pomembni za zanesljivo kvalitativno in kvantitativno določitev, kot so: vzorčenje in izbira reprezentitativnega vzorca, priprava vzorca, specifičnost analitske metode in kritično vrednotenje rezultatov.

V monografiji »Modern extraction techniques for essential oils«, smo objavili prispevek v katerem so opisane sodobne ekstrakcijske tehnike za eterična olja (*AL33*). Eterična olja so v farmakopejah definirana kot hlapne sestavine rastlin, ki jih izoliramo s hidrodestilacijo (HD), parno destilacijo (SD) ali stiskanjem. Za bolj občutljiva eterična olja se uporablja ekstrakcija s topili (SE). Pomanjkljivosti teh standardnih tehnik so dobro poznane: izguba hidrofilnih in termično labilnih spojin pri HD/SD, okoljsko problematična in draga topila, precejšnja poraba časa in energije. Sodobne uveljavljene in nove ekstrakcijske tehnike stremijo k preseganju teh težav. V pričujočem pregledu, ki povzema pretežno znanstvene prispevke zadnjega desetletja, je podana razprava o njihovih prednostih, slabostih in uporabnosti.

Raziskave povezane z analitiko v industriji, smo v sodelovanju z LEKom nadaljevali na področju določanja nečistoč v zdravilih. Predvsem smo se ukvarjali z identifikacijo številnih nečistot v gentamicinu. Ta problematika je zelo zahtevna saj lahko nečistote v gentamicinu identificiramo samo z zahtevnimi detekcijskimi sistemi kot je tandemska masna spektrometrija. S kombinacijo ionsko parne kromatografije in tandemske masne spektometrije smo uspeli na kromatogramu gentamicina poleg štirih glavnih komponent gentamicina identificirati še 17 nečistoč, kot je to opisanov članku objavljenem v *J. Pharm. Biomed. Anal*. (*AL21*) in v doktorski disertaciji (COBISS.SI-ID 248182016).

V okviru raziskav in razvoja metod za analitiko živil, smo v članku, objavljenem v reviji *Acta Chim. Slov.* (*AL19*) opisali prilagojeno standardno metodo SIST EN 1528 1–4: 1998: Metoda D, ki je primerna za določevanje organokloriranih pesticidov (OCP) v mesnih prehrambenih izdelkih. Glavne spremembe so bile napravljene v stopnji ekstrakcije, kjer smo hladno ekstrakcijo nadomestili s Soxhlet ekstrakcijo. Za čiščenje vzorcev predlagamo uporabo manjših kolon, za koncentriranje analitov pa smo namesto tehnike izparevanja topila z rotavaporjem uporabili Kuderna-Danish koncentratorje. Vpeljane spremembe so pripomogle k izboljšanju izkoristkov za vzorce z visoko vsebnostjo maščob, ki so bili za vse analizirane pesticide nad 60 %. Natančnost postopka, izražena kot relativni standardni odmik, je bila 10 %. Metoda je primerna za določevanje OCP v mesnih izdelkih z visoko vsebnostjo maščob. Meje zaznav za OCP so bile v območju od 0,1 ppb za lindan ter 2 ppb za α-endosulfan.

Med snovi, ki so pomembne za obstojnost in stabilizacijo živil, sodijo tudi naravni antioksidanti. Običajna razdelitev fenolnih antioksidantov je na flavonoidne in neflavonoidne antioksidante. Glede na taninski karakter jih lahko delimo tudi na taninske in netaninske fenole. Posledica vsebnosti teh spojin v vinu je njihova visoka antioksidativna kapaciteta. V raziskavi smo določevali galno kislino, katehin, epikatehin, resveratrol, kvercetin, dihidroksibenzojsko kislino, sinapično kislino, kavno kislino, klorogensko kislino, ferulno kislino, elaginsko kislino, p-kumarinsko kislino in kaftarno kislino v 141 vzorcih vina s tekočinsko kromatografijo (z masnospektrometrično detekcijo in UV detekcijo). Skupno antioksidativno učinkovitost smo določali tudi z metodo po Folin-Ciocalteu-ju. Kljub zadovoljivi korelaciji med obema metodama, smo opazili statistično pomembne razlike med določitvami s spektrofotometrično metodo in z metodo LC/MS/MS, in sicer so ujemanja med obema metodama različna za rdeča, bela in rosé vina, kot je to podrobneje opisano v članku, objavljenem v reviji *Acta Chim. Slov.* (*AL1*).

Odziv monoterpenske sestave vina traminec (*Vitis vinifera* L.) na različne encimske pripravke, je opisan v članku objavljenem v *Afr. J. Enol. Vitic.* (*AL17*). V grozdju, moštu in vinu sorte traminec, smo po obdelavi s šestimi različnimi pektolitičnimi encimi [Lallzyme-β (‘Lall’); Rohavin VR-C (‘VRX’), Rohapect D5L (‘D5L’), Rohavin MX (‘MX’), Rohapect VRC (‘VRC’), Endozym cultivar A (‘Cult. A’)] in z β-glukozidazo (βG, EC 3.2.1.21) določali poglavitne aromatične monoterpene α-terpineol, linalool, nerol in geraniol. Koncentracije monoterpenskih spojin smo določali z mikroekstrakcijo na trdno fazo (SPME) in GC-MS. V grozdju sorte traminec je bila najvišja vsebnost monoterpena geraniola (66,7 μg/L), sledili so mu nerol (13,3 μg/L), α-terpineol (7,8 μg/L) in končno linalool (3,3 μg/L). Najbolj aromatično vino traminec je nastalo iz mošta, obdelanega z encimskim preparatom ‘Lall’, kar smo potrdili s senzorično in kemijsko analizo, s katero smo določili koncentracijo nerola (45,9 μg/L), geraniola (31,8 μg/L), α-terpineola (10,5 μg/L) in linaloola (6,1 μg/L). Pokazalo se je, da so vina, narejena iz encimatsko obdelanega mošta, imela višjo koncentracijo monoterpenskih spojin v primerjavi s kontrolo, čeprav senzorična analiza tega ni prepričljivo potrdila.

Članek, objavljen v reviji *Food Chemistry* (*AL18*), obravnava problematiko identifikacije spojin arome ajde (*Fagopyrum esculentum* Moench). Ajda ima močno in karakteristično aromo, vendar njeno fitokemijsko ozadje še ni docela dognano. Namen te študije je bil identifikacija in kvantifikacija posameznih spojin, ki so odgovorne za aromo ajde. Hlapne spojine iz sveže zmlete ajdove moke smo ekstrahirali z različnimi metodami: direktna ekstrakcija s petroletrom, pentanom ali metanolom, destilacija s Clevengerjevim aparatom in mikroekstrakcija na trdno fazo iz plinske faze nad vzorcem. Ekstrakte smo analizirali z GC–MS z elektronsko ionizacijo. Spojine smo identificirali z MS in s primerjavo retencijskih časov z referenčnimi spojinami. Kot zelo učinkoviti sta se izkazali direktna ekstrakcija z metanolom in destilacija. V teh dveh ekstraktih smo identificirali petindvajset oziroma petintrideset spojin. Metanolni ekstrakt je vseboval bolj hidrofilne, destilacijski pa bolj hlapne spojine. Večino spojin smo kvantificirali in jim izračunali aktivnost vonja (OAV). V obeh ekstraktih hkrati sta se nahajali samo dve spojini: salicilaldehid in fenilacetaldehid. Spojine, ki največ prispevajo k aromi ajde, so 2,5-dimetil-4-hidroksi-3(2*H*)-furanon, (*E,E*)-2,4-dekadienal, fenilacetaldehid, 2-metoksi-4-vinilfenol, (*E*)-2-nonenal, dekanal, heksanal in salicilaldehid (2-hidroksibenzaldehid).

V okviru raziskav povezanih z okoljsko problematiko, smo v sodelovanju z raziskovalci BTF razvijali okolju prijazne premaze za zaščito lesa, med katere spadajo premazi, ki vsebujejo borovo kislino. Glavna težava pri uporabi borovih spojin, sicer zelo učinkovitih fungicidov in insekticidov, je njihovo izpiranje iz lesa. Borovo kislino smo kombinirali z emulzijo montanskega voska, ki sodi med sredstva za povečevanje vodoodbojnosti lesa. Neimpregnirani in impregnirani vzorci smrekovega in bukovega lesa so bili 12 tednov izpostavljeni glivam razkrojevalkam (*Trametes versicolor*, *Pleurotus ostreatus*, *Hypoxylon fragiforme*, *Gloeophyllum trabeum*, *Antrodia vaillantii* in *Serpula lacrymans*). Rezultati fungicidnih testov kažejo na sinergistični učinek obeh zaščitnih pripravkov. Pri kombinaciji borove kisline in montanskega voska dosežemo ustrezno zaščito lesa že z nižjimi koncentracijami borove kisline, prav tako pa se izpiranje borove kisline zmanjša za 20 do 50 %, kot je to opisano v članku, objavljenem v reviji *International Biodeterioration & Biodegradation* (*AL10*).

# RESEARCH PROGRAMME REPORT

## RESEARCH TOPICS AND GOALS

a) Basic research of 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 the year 2009 members of the programme group published 21 original scientific articles (*AL1-21*), one review article (*AL22*), delivered two invited lectures (*AL23-24*), six lectures on scientific conferences (*AL25-30*) and published three contributions in scientific monographs (*AL31-33*). The results of the research were presented also at numerous scientific conferences.

The following subjects were studied:

**a)**

Ion attachment mass spectrometry (IAMS) is combined with an in-house single-atom infrared image furnace (IIF) for thermal analysis studies. Besides the detection of many chemical species at atmospheric pressure, including free radical intermediates, the ion attachment mass spectrometer can also be used for the analysis of products emanating from temperature-programmed pyrolysis. The performance and applicability of the IIF-IAMS is illustrated with poly(tetrafluoroethylene) (PTFE) samples. Temperature-programmed decomposition of PTFE gave constant slopes of the plots of temperature versus signal intensity in a defined region and provided an apparent activation energy of 28.8 kcal/mol for the PTFE decomposition product $(CF_2)_3$. A brief comparison with a conventional pyrolysis GC/MS system is also given. The article is published in distinguished journal *Analytical Chemistry* (*AL3*).

In the article published in *Journal of Physical Chemistry A* (*AL14*) density functional theory was used to calculate the proton affinity and to determine the global minimum energy structures of fullerene ($C_{60}$) and its protonated forms. Vibrational frequency calculations were used to check the nature of these predicted structures. In the protonation of $C_{60}$ in the gas phase, the proton preferentially lies above carbon atoms at a distance of 1.10 Å, which suggests a bond of covalent nature. The proton affinity for fullerene was calculated as 201.8 kcal/mol, compared with the experimental value between 204 and 207 kcal/mol obtained by proton-transfer bracketing studies using Fourier transform mass spectrometry. All five transition states for intramolecular proton transfer in fullerene were found, three for the first time. The activation energy ($E_a$) barriers for proton migration were calculated and ranged from 27 to 90 kcal/mol. Different functional groups attached to fullerenes, and their influence on *E*a values are discussed, as possible proton transfers for nonfunctionalized fullerenes.

In our paper entitled "Material degradomics: on the smell of old books" published in *Analytical Chemistry* (*AL4*) we successfully transferred and applied -omics concepts to the study of material degradation, in particular historic paper. The main volatile degradation products of paper, which form a typical "smell of old books", were determined using headspace analysis after a 24 h predegradation procedure. Using supervised and unsupervised methods of multivariate data analysis, we were able to quantitatively correlate volatile degradation products with the properties important for the preservation of historic paper: rosin, lignin and carbonyl group content, degree of polymerization of cellulose, and paper acidity. On the basis of volatile degradic footprinting, we identified degradation markers for rosin and lignin in paper and investigated their effect on degradation. Apart from the known volatile paper degradation products acetic acid and furfural, we also proposed a number of other compounds of potential interest, most notably lipid peroxidation products. The nondestructive approach can be used for rapid identification of degraded historic objects on the basis of volatile degradation products emitted by degrading paper.

Investigation of the mechanism of copper dissolution in strong ammonia solutions is described in the article published in the *Journal of the The Electrochemical Society* (*AL15*). Corrosion of copper in ammonia solutions is significantly affected by many parameters such ammonia concentration , pH, temperature, concentration of $Cu^{2+}$, the presence/absence of dissolved oxygen, the chemical nature, and the concentration of the anion but also by selected corrosion products, in particular, $Cu^{+}$, various adsorbed intermediates, and finally passive films. In this work we tried to elucidate the corrosion of copper in a wide potential window and in a broad range of concentrations of various species (0.2–3.5 mol/L $NH_3$, 0–0.1 mol/L $Cu^{2+}$, pH 10–12.5). We focussed on the first peak occurring within −1.0 to −0.6 V vs MSE with the aim to explain the underlying mechanism. We show that the reaction order of the dissolution reaction with respect to ammonia is 2. We further show that using conventional electrochemical methods in combination with an optical method (scanning electron microscopy), a two-step electrochemical-chemical) reaction yielding $Cu_2O$ is identified as the most likely passivation mechanism, confirmed also by performing impedance analysis at various experimental conditions.

Response behaviour of amperometric glucose biosensors based on different carbon substrate transducers coated with enzyme-active layer was investigated and published in *Electroanalysis* (*AL20*). Carbon electrodes (glassy carbon, GC, screen-printed carbon, SPC, and carbon fiber, CF) were used as substrate transducers to prepare glucose biosensors of different sizes and geometries, based on ruthenium hexacyanoferrate as $H_2O_2$ reduction mediator and glucose oxidase immobilized in a poly(1,2-phenylenediamine) membrane. Their response behavior under hydrodynamic amperometric conditions at an operating potential of –0.02 V vs. Ag/AgCl was studied and compared. We found that the GC and SPC biosensors showed enzymatic catalysis controlled current response with nonlinear concentration dependence, while the CF based micro-biosensor exhibited diffusion-controlled current response, extended linear range calibration curves with relatively lower sensitivity and longer response times.

Development of a reliable method for plutonium isotope ratio measurements is the subject of the paper published in *International Journal of Mass Spectrometry* (*AL11*). A sample preparation procedure for isotopic measurements using thermal ionization mass spectrometry (TIMS) was developed which employs the technique of carburization of rhenium filaments. Carburized filaments were prepared in a special vacuum chamber in which the filaments were exposed to benzene vapour as a carbon supply and were electrothermally carburized. To find the optimal conditions for the carburization and isotopic measurements using TIMS, the influence of various parameters such as benzene pressure, carburization current and the exposure time were tested. As a result, carburization of the filaments improved the overall efficiency by one order of magnitude. Additionally, a new “multi-dynamic” measurement technique was developed for Pu isotope ratio measurements using a “multiple ion counting” (MIC) system. This technique was combined with filament carburization and applied to the NBL–137 isotopic standard and samples of the NUSIMEP 5 inter-laboratory comparison campaign, which included certified plutonium materials at the ppt-level. The multi-dynamic measurement technique for plutonium, in combination with filament carburization, has been shown to significantly improve the precision and accuracy for isotopic analysis of environmental samples with low-levels of plutonium.

In the study published in *Environmental Chemical Letters* (*AL9*), stability of statin drugs in different conditions, such as various pH, diverse solvents ratio, presence of UV, and sunlight have been investigated. 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 p–p* band. In acidic conditions the interconversion between lactone and hydroxy acid forms in aqueous solutions at room temperature is retarded, while in sun-exposed samples it is accelerated. Longer exposures lead to degradation. Statin interconversion in water is much lower than in acetonitrile.

Development and characterization of methacrylate-based hydrazide monoliths for oriented immobilization of antibodies was investigated and published in the *Journal of Chromatography A* (*AL12*). Convective interaction media (CIM, BIA Separations) monoliths are attractive stationary phases for use in affinity chromatography because foster affinity binding, which is a consequence of convectively enhanced mass transport. This work focuses on the development of novel CIM hydrazide (HZ) monoliths for the oriented immobilization of antibodies. Adipic acid dihydrazide (AADH) was covalently bonded to CIM epoxy monoliths to form hydrazide groups on the monolith surface. Two different antibodies were afterwards immobilized to hydrazide functionalized monolithic columns and thus prepared columns were tested for their selectivity and dynamic binding capacity.

Human serum albumin (HSA) and immunoglobulin G (IgG) represent over 75% of all proteins present in human plasma. These high-abundance proteins prevent the detection of low-abundance proteins which are potential markers for various diseases. The depletion of HSA and IgG is therefore essential for further proteome analysis. In this paper we describe the optimization of conditions for selective depletion of HSA and IgG using affinity and pseudo-affinity chromatography. A BIA Separations CIM (convective interaction media) Protein G disk was applied for the removal of IgG and the Mimetic Blue SA A6XL stationary phase for the removal of HSA. The binding and the elution buffer for CIM Protein G disk were chosen on the basis of the peak shape. The dynamic binding capacity was determined and it was shown that it depends on the buffer system used while it is independent from the flow rate and concentration of IgG. Beside the binding capacity for the IgG standard, the binding capacity was also determined for IgG in human plasma. The Mimetic Blue SA A6XL column was characterized using human plasma. The selectivity of the depletion depended on the amount of human plasma that was loaded on the column. After the conditions on both supports had been optimized, the Mimetic Blue SA A6XL stationary phase was combined with the CIM Protein G disk in order to simultaneously deplete samples of human plasma. A centrifuge spin column that enables the removal of IgG and HSA from 20 µL of human plasma was designed. The results of the depletion were examined using sodium dodecyl sulfate polyacrylamide gel electrophoresis and two-dimensional gel electrophoresis. Results of this research were published in the *Journal of Chromatography A* (*AL13*).

Detailed uncertainty budget for major and minor ions in calibration standards were investigated and published in *Analytica Chimica Acta* (*AL2*). A general methodology for a systematic evaluation of the uncertainty was derived 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 recognizing the major contributions to combined uncertainties. This work confirmed that it is justifiable to take into account the mass fraction of impurities in other chemicals when calculating the mass concentration of an ion in combined calibration standard solution similarly to what is already a common practice in accounting for the purity of a chemical. It was proven that impurities in chemicals which are sources of major ions have significant effects on uncertainty budget of minor ions; even 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.

**b)**

Historic parchment is a macromolecular material, which is complex due to its natural origin, inhomogeneity of the skin structure, unknown environmental history and potential localised degradation. In the article published in *Polymer Degradation and Stability* journal (*AL16*) autoxidation of lipids in parchment was investigated. By gas-chromatographic analysis of the atmosphere surrounding parchment during oxidation, we provide the experimental evidence on the production of volatile aldehydes, which can be the products of lipid peroxidation. Oxidation of parchment with different aldehyde emissions was additionally followed in situ using chemiluminometry and the same technique was used to evaluate the oxidation of differently delipidised parchment. It was shown that the production of peroxides in the material decreases with lower lipid content. Drawing upon this evidence we can conclude that the presence of lipids (either initially present in the skin, added during production or conservation) leads to oxidative degradation of collagen and that the non-destructive analysis of emission of volatiles could be used as a quick tool for the evaluation of parchment stability.

Wood pulp cellulose was used in studying catalyzed liquefaction in the presence of ethylene glycol, p-toluene sulfonic acid monohydrate or sulphuric acid acting as the catalysts. For this study, microcrystalline cellulose, Whatman filter paper and cotton linters with molar masses of 76,000, 699,000 and 1,910,000 g mol/1, respectively were used. This liquefaction was studied by gravimetric determinations, by X-ray diffraction analysis of the residual cellulose and by monitoring the molar mass decrease over different time intervals, using size-exclusion chromatography. The disordered regions, even of cellulose with the highest molar mass, degraded in the initial minute of liquefaction. However, the highly ordered cellulose regions remained relatively stable for a longer time. Nonetheless, partial degradation of the highly ordered regions of the cellulose was achieved as described in the paper published in *Cellulose* (*AL7*).

The mechanism of duplex stainless steel oxidation by oxygen was investigated in detail and the results were published in journals *Applied Surface Science* (*AL5*) and *Corrosion Science* (*AL8*). Three different techniques were used to produce thin oxide layers on polished and sputter-cleaned duplex stainless-steel (DSS) alloy 2205 samples. These samples were exposed to $10^{-5}$ mbar of pure oxygen inside the vacuum chamber, exposed to ambient conditions for 24 h, and plasma oxidized. The oxide layers thus produced were analyzed using XPS depth profiling in order to determine the oxide layers' compositions with depth. We found that all the techniques produce oxide layers with different traces of metallic components and a common characteristic of all the oxide layers investigated is a double-oxide stratification, with regions closer to the surface exhibiting higher concentrations of iron oxide, and those more in-depth exhibiting higher concentrations of chromium oxide. Surface oxidation of the duplex stainless steel was studied by X-ray photoelectron spectroscopy (XPS) and SEM imaging. The experiments were performed on the alloy after controlled oxidation with oxygen atoms created in an inductively coupled plasma and at temperature ranges from room temperature up to 700 ºC. Compositions of the modified oxidized surfaces were obtained from XPS survey scans, and the chemistries of selected elements from higher energy resolution scans of appropriate peaks.

The morphologies of the surfaces were obtained using field emission scanning electron microscopy at different magnifications, up to 10,000 x. Different Fe/Cr/Mn oxidized layers and oxide thicknesses were observed and correlated with temperature. This subject is also a part of a doctoral thesis (COBISS.SI-ID 30608133).

Self-crosslinking and film formation ability of liquefied black poplar were investigated and published in *Bioresource Technology* (*AL6*). Black poplar wood, diethylene glycol (DEG), and sulphuric acid as a catalyst were used as starting reactants for liquefaction. Optimal conditions for liquefaction were established: reaction temperature 150 ºC, reaction time 95 min, ratio of wood: DEG = 1:5 and 3% of sulphuric acid addition. The liquid mixture obtained by the liquefaction was composed of the real product of the reaction (the so called ‘‘excess solvent free liquefied wood” (ESFLW)) and of the remaining unreacted DEG. The unreacted DEG was successfully separated from the ESFLW and analyzed with HPLC for levulinic acid content. Theoretical weight ratio between the wood and DEG required for the reaction was estimated. OH number investigation showed that the ESFLW in the liquid mixture contributes to maximum 60% of the free AOH groups. The crosslinking of the ESFLW without any curing agents or additives was performed for the first time, and the drying stages investigated. FT-IR investigations demonstrated that the obtained crosslinked polymer film could be an ether and/or ester network.

**c)**

In the article published in *International Journal of Molecular Sciences* (*AL22*) conventional and emerging analytical methods for the determination of mycotoxins were reviewed and discussed. An overview of methods for the analysis and sample preparation published in the last ten years is given for the most often encountered mycotoxins in different samples, mainly in food. Special emphasis is on liquid chromatography with fluorescence and mass spectrometric detection, while in the field of sample preparation various solid-phase extraction approaches are discussed, and an overview of other analytical and sample preparation methods less often used is also given. Finally, different matrices where mycotoxins have to be determined are discussed with the emphasis on their specific characteristics important for the analysis (human food and beverages, animal feed, biological samples, environmental samples). Various issues important for accurate qualitative and quantitative analyses are critically discussed: sampling and choice of representative sample, sample preparation and possible bias associated with it, specificity of the analytical method and critical evaluation of the results.

Modern extraction techniques for essential oils and aromas were presented in a scientific contribution of a monograph (*AL33*). Essential oils are defined in the pharmacopoeias as volatile constituents of plants separated by hydrodistillation (HD), steam distillation (SD) or pressing. Solvent extraction (SE) is used for more delicate essential oils. The drawbacks of these standard techniques are well recognized: loss of hydrophilic and thermally labile compounds in HD-SD, environmentally problematic and expensive solvents, significant consumption of time and energy. Modern established and emerging extraction techniques for essential oils aim to overcome these problems. Their advantages, disadvantages and applicability are discussed in this review, which covers mainly the scientific literature published in the last decade.

An HPLC/MS/MS method was developed for identification of impurities in gentamicin and published in *J. Pharm. Biomed. Anal*. (*AL21*). The HPLC was performed on a Synergy Hydro-RP column using 50mM trifluoroacetic acid (TFA), pH 2 adjusted with ammonium solution and methanol as mobile phase. All impurities in gentamicin were separated from main gentamicin components. Atmospheric pressure chemical ionization (APCI) was used and product mass spectra of protonated molecules were acquired. Seventeen impurities were detected in gentamicin. Reference compounds: gentamicins: $C_{2b}$, B, $B_1$, G–418, sisomicin, garamine and gentamines: $C_1$, $C_{1a}$, $C_2$, $C_{2a}$ were used for spectra interpretation and impurities identification. All MS/MS spectra were interpreted and fragmentation transitions for gentamicins and in general for aminoglycoside antibiotics (AG) were proposed.

In the paper published in *Acta. Chim. Slov*. (*AL19*) the modification of standard method SIST EN 1528 1–4: 1998: Method D for measurements of organochlorine pesticides (OCPs) in food products is presented. The modifications were made in the extraction step in which cold extraction technique was replaced by Soxhlet extraction. For the clean-up step smaller columns were introduced and in the concentration step rotary evaporation was replaced by Kuderna-Danish concentration technique. Thus introduced modifications improved the efficiency of the procedure for samples with high fat content. Recovery values for all analyzed pesticides were over 60% and the reproducibility expressed as relative standard deviation was in the range of 10%. The method is suitable for the determination of OCPs in meat products with high content of fat from low ppb concentration range onward. The limits of detection for examined OCPs were in the range from 0.1 ppb to 2 ppb for lindane and α-endosulfan, respectively.

Comparison of methods for determination of polyphenols in wine by HPLC-UV/VIS, LC/MS/MS and spectrophotometry were investigated and published in *Acta Chim. Slov.* (*AL1*). Phenolic antioxidants are usually grouped into flavonoids and non-flavonoids, and to tannic phenols and non-tannic phenols. Collectively, these compounds contribute to high antioxidant capacity of wine. In this work, we compare the determination of gallic acid, catechin, epicatechin, resveratrol, quercetin, dihydrobenzoic acid, sinapic acid, vanillic acid, caffeic acid, chlorogenic acid, ferullic acid, ellagic acid, *p*-coumaric acid and caftaric acid in 141 wine samples using two liquid chromatographic methods and detection systems, i.e. by UV detection and mass-spectrometric detection. In addition, we applied the conventional Folin-Ciocalteu spectrophotometric method for determination of the total phenolic content in wine samples and compared the results with those obtained using the chromatographic methods. Despite satisfactory correlations statistically significant differences between HPLC-UV/VIS and LC/MS/MS were established, which could be related to coelution not detectable by UV/VIS detectors. The correlations between the results of the spectrophotometric method and the sum of LC/MS/MS determinations are not satisfactory and are different in white, red, and rosé wines.

The response of monoterpenes to different enzyme preparations in wines were investigated and published in *S. Afr. J. Enol. Vitic* (*AL17*). The α-terpineol, linalool, nerol and geraniol, which are the main aromatic monoterpenes in the grapevine variety Gewürztraminer, were determined in the grapes, in must and in wine after a treatment with six different pectolytic enzymes [Lallzyme-β ('Lall'); Rohavin VR-C ('VRX'), Rohapect D5L ('D5L'), Rohavin MX ('MX'), Rohapect VRC ('VRC'), Endozym cultivar A ('Cult. A')], and after treatment with β-glucosidase (βG, EC 3.2.1.21). The concentrations of monoterpenic compounds were determined by solid-phase microextraction (SPME) and GC-MS. The most abundant monoterpene in the grapes of Gewürztraminer was geraniol (66.7 μg/L), followed by nerol (13.3 μg/L), α-terpineol (7.8 μg/L) and finally linalool (3.3 μg/L). Gewürztraminer wine produced from the must treated with the Lall enzyme preparation was the most aromatic, which was also confirmed by chemical and sensory analysis in which the concentrations of nerol (45.9 μg/L), geraniol (31.8 μg/L), α-terpineol (10.5 μg/L) and linalool (6.1 μg/L) were determined. The wines produced from the must chemically treated with enzymes showed higher concentrations of many of the monoterpene compounds compared to the control sample, although the sensorial analysis did not confirm this convincingly.

Buckwheat (*Fagopyrum esculentum Moench)* has a strong and typical aroma, but its phytochemical background has not been fully elucidated yet. The aims of this study published in *Food Chemistry* (*AL18*) was to identify and quantify individual compounds responsible for the buckwheat aroma. Volatiles from freshly ground buckwheat flour were extracted by different methods: direct extraction with petroleum ether, pentane or methanol, distillation with Clevenger apparatus and a headspace solid-phase microextraction method. The extracts were analysed by GC–MS with electron ionisation. Compounds were identified by MS and by comparison of retention times with reference compounds. Direct extraction with methanol and distillation proved to be very efficient. In these extracts twenty-five and thirty-five compounds were identified, respectively. The first extract contained more hydrophilic compounds and the latter more volatile compounds. Most of the compounds were quantified and their odour activity value (OAV) calculated. Only two compounds (salicylaldehyde and phenylacetaldehyde) were found in both extracts. The compounds with the highest contribution to the buckwheat aroma were: 2,5-dimethyl-4-hydroxy-3(2H)-furanone, (E,E)-2,4-decadienal, phenylacetaldehyde, 2-methoxy-4-vinylphenol, (E)-2-nonenal, decanal, hexanal and salicylaldehyde (2-hydroxybenzaldehyde).

In the article published in *Int. Biodeterioration and Biodegradation* journal (*AL10*), improvement of performance of boron-based wood preservatives were presented. The importance of boron compounds in wood preservation is increasing due to their low environmental impact, high efficacy and the fact that many other active ingredients have been removed from the market after introducing the Biocidal Products Directive. The most important drawback of boron is prominent leaching in wet environment. In order to improve fixation of ingredients, and performance against wood decay fungi, boric acid was combined with montan wax emulsion. Possible synergistic effects of boric acid and montan wax were determined according to modified EN 113 procedure. Norway spruce and beech wood specimens were exposed to tree white rot (*Trametes versicolor*, *Pleurotus ostreatus* and *Hypoxylon fragiforme*) and brown rot wood decay fungi (*Gloeophyllum trabeum*, *Antrodia vaillantii* and *Serpula lacrymans*) for 12 weeks. Boron leaching from vacuum/pressure treated Norway spruce wood was determined by continuous (EN 84 and ENV 1250–2) and non-continuous (OECD and prCEN/TS 15119–1) procedures. Boron was determined by ICP mass spectrometry in collected leachates. The results of the fungicidal tests clearly showed that montan wax emulsion and boric acid act synergistically against tested wood decay fungi. Approximately 50 % lower boric acid retentions are required in combination with montan wax emulsions to achieve sufficient protection against wood rotting fungi. However, it is even more important that all leaching tests performed proved that the addition of montan wax decreased boron leaching from impregnated specimens by 20 % up to 50 %.

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

### PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

**P1–0175**

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# POROČILO O REALIZACIJI PROGRAMA

## CILJI PROGRAMA

Vsebino raziskovalnega programa lahko razdelimo v dva sklopa. Prvi sklop se ukvarja z bazičnimi raziskavami, drugi sklop pa naj bi bil bolj usmerjen v aplikativne raziskave. V okviru programa bomo raziskovali pogoje priprave različnih spojin, anorganskih koordinacijskih in organokovinskih spojin z različnimi ligandi. Kemijsko čiste produkte bomo karakterizirali z različnimi fizikalno-kemijskimi metodami in določali bomo njihovo biološko učinkovitost. Podoben postopek bomo 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.

## OSREDNJE TEME PROGRAMA

Osrednje teme programa so večplastne. V okviru programske skupine so bomo predvsem ukvarjali z:

**Kinoloni.** V zadnjih letih so kinoloni postali najuspešnejša klinično uporabljena protibakterijska sredstva (ciprofloxacin kot »blockbuster drug«). Naš namen je bil pripraviti nove komplekse kovin in kinolonov ter preučevati njihove fizikalno-kemijske lastnosti. Med časom trajanja se bomo začeli ukvarjati tudi z interakcijami kovinskih ionov s triazoli, ki tudi imajo biološko aktivnost.

**Sinteza in karakterizacija lantanoidnih kompleksov.** Lantanoidi so zanimivi zaradi svojih posebnih lastnosti: reaktivnosti, topnosti v organskih topilih, fluorescence, katalitskih, optičnih in magnetnih lastnosti in se lahko uporabljajo v raziskavah in proizvodnji. V organskih reakcijah lahko sodelujejo kot izhodne spojine zaradi svoje reaktivnosti in topnosti v organskih topilih. Sintetizirali bomo komplekse lantanoidnih halogenidov iz lantanoidnih oksidov in lantanoidnih halogenidov hidratov s preprostejšimi O- in N-donorskimi ligandi.

**Osnovni organokovinski fluoridi.** Organokovinski fluoridi s ciklopentadienilnim ligandom so katalitično aktivni za reakcije polimerizacije (npr. za stereospecifično pripravo polistirena). Raziskave bomo razširili na področje ciklooktatetraenilnih kloridov in fluoridov Ti, Zr, Hf in lantanoidov, pri katerih pričakujemo podobne katalitične aktivnosti. V prvi stopnji bo izveden sintezni del in rentgenska strukturna analiza.

**Supramolekularne strukture in gost-gostitelj vgraditve: primer organokovinskih fluoridov:** V okviru projekta bomo raziskali vpliv vodikovih vezi na kristalno arhitekturo organokovinskih fluoridov. Vodikove vezi tipa M–F···H–N sodijo med močne vodikove vezi, ki so na področju fluorokemije malo raziskane. Posebna pozornost bo namenjena neklasičnim, šibkim vodikovim vezem tipa M–F···H–C (npr. z $CH_2Cl_2$, $CHCl_3$ …), ki predstavljajo novo, atraktivno področje supramolekularne kemije.

**Zaščitna sredstva za les.** Ta sredstva za les se v velikih količinah uporabljajo v komercialne namene že več desetletij. V pripravkih so prisotni tudi zelo strupeni dodatki (krom in arzen), saj pomembno vplivajo na učinkovito protibiološko zaščito lesa ter preprečujejo izpiranje sredstev z zaščitene površine. Okoljsko najbolj obremenjujoči dodatki bodo zelo verjetno kmalu prepovedani. Zaradi tega je potrebno razviti novo generacijo zaščitnih sredstev za les. Poseben poudarek je potreben za močnejšo vezavo/slabše izpiranje na/z tako zaščitene lesne površine.

**Strukturno delo.** V okviru programske skupine skrbimo in bomo še naprej skrbeli za razvoj znanosti o strukturi snovi tako z metodološkega kot teoretskega stališča. Po eni strani je to potrebno zato, ker bo sama strukturna karakterizacija ključna zahteva za večino snovi, ki bodo sintetizirane v predlaganem programu, po drugi pa je potrebno spremljati in dopolnjevati znanje o povezanosti zgradbe snovi in njenih lastnosti. Obseg tega znanja v svetu v zadnjem času hitro narašča, saj je temeljnega pomena za načrtovano določanje oz. spreminjanje lastnosti snovi. Ukvarjali se bomo s kombinacijo praškovne kristalografije in kvantnokemijskih računov. Ker smo bili v preteklem obdobju na tem področju v koraku s svetom, želimo to nadaljevati in utreti pot souporabi teh dveh metod tudi na področje mikrovalovne keramike, kjer bodo rezultati nedvomno zanimivi.

**Novi materiali.** Razvoj znanosti in gospodarstva zahteva nagle odgovore, podporo z raziskavami in razvojem novih materialov s široko paleto lastnosti ter na njihovi osnovi zasnovane uporabnosti takih materialov.

Področje priprave oziroma sinteze novih materialov je že vrsto let v ospredju različnih raziskovalnih programov. Stihijski razvoj različnih metod je v novejšem času zamenjal bolj načrtovan pristop, ki pri razvoju nove metode upošteva vrsto pogojev: dostopnost surovinske osnove po sprejemljivih cenah, razpoložljivost opreme, možnost za povečevanje kapacitet do malotonažnega nivoja ali celo preko tega, okoljska sprejemljivost metode, kriteriji ekonomske uspešnosti metode ali procesa pri prenosu v večje merilo.

Izbor materialov oziroma njihovih kombinacij pri kompozitnih materialih je usmerjen v katalizatorje in elektrokatalizatorje. Prevladujoča integracija katalizatorjev v kemijske procese na področju sinteze različnih produktov, sodobnih in alternativnih virov električne energije in pri procesih za ohranjanje naravnega okolja, vodi naše aktivnosti v tej smeri.

## ZNANSTVENI DOSEŽKI

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

### RED/NERED KISIKOVIH ANIONOV

Z Rietveld piljenjem sedmih spojin s formulami $La_2Ti_{(1-x)}Ga_xO_{(5-x/2)}$, kjer je $x = 0.00$, 0.20, 0.50, 0.70, 0.90, 0.95 and 1.00, smo uspešno opisali topnost v trdnem stanju med $La_2TiO_5$ in $La_4Ga_2O_9$. Opisana je tudi podobnost obeh struktur.

- KASUNIČ, Marta, MEDEN, Anton, ŠKAPIN, Srečo D., SUVOROV, Danilo, GOLOBIČ, Amalija. Order-disorder of oxygen anions and vacancies in solid solutions of La[sub]2 TiO[sub]5 and La[sub]4Ga[sub]2O[sub]9. *Acta crystallogr., B Struct. sci.*, 2009, vol. B65, no. 5, str. 558–566. [COBISS.SI-ID 30821637]

## MAGNETNA SKLOPITEV MED BAKROVIMI(II) IONI

Nova dinuklearna bakrova(II) koordinacijska spojina je bila sintetizirana s pomočjo liganda Schiffove baze. Merjenje magnetne susceptibilnosti do 3 K je pokazalo, da sta dva kovinska iona antiferomagnetično sklopljena. Razlog za to naj bi bila vodikova vez.

- TANG, Jinkui, COSTA, José Sánchez, GOLOBIČ, Amalija, KOZLEVČAR, Bojan, ROBERTAZZI, Arturo, VARGIU, Attilio V., GAMEZ, Patrick, REEDIJK, Jan. Magnetic coupling between copper(II) ions mediated by hydrogen-bonded (neutral) water molecules. *Inorg. chem.*, 2009, vol. 48, no. 12, str. 5473–5479. [COBISS.SI-ID 30579205]

## BAKROVI(II) KOORDINACIJSKI POLIMERI

Opisane so sinteza, strukturna kemija in magnetne lastnosti vrste novih bakrovih(II) koordinacijskih polimerov z dikarboksilnimi kislinami. Obstajajo kot linearne verige ali pa so dvodimenzionalno povezani.

- LAH, Nina, CLÉRAC, Rodolphe. Cu(II) coordination polymers incorporating 3-aminopyridine and flexible aliphatic dicarboxylate ligands : synthesis, structure and magnetic properties. *Polyhedron*. [Print ed.], 2009, vol. 28, no. 12, str. 2466–2472. [COBISS.SI-ID 30716165]

## BAKROVI(II) KOMPLEKSI Z MALIMI METANOATNIMI LIGANDI

Bakrovi(II) metanoatni kompleksi so lahko mononuklearni, binuklearni ali polinuklearni. Okarakterizirani so bili z različnimi fiziko-kemijskimi metodami.

- KOZLEVČAR, Bojan, MATE, Elizabeta, JAGLIČIĆ, Zvonko, GLAŽAR, Lea, GOLOBIČ, Amalija, STRAUCH, Peter, MONCOL, Jan, KITANOVSKI, Nives, ŠEGEDIN, Primož. A small methanoato ligand in the structural differentiation of copper(II) complexes. *Polyhedron*. [Print ed.], 2009, vol. 28, no. 13, str. 2759–2765. [COBISS.SI-ID 30678021]

## NIZKOTEMPERATURNA SINTEZA BAKER/CINKOVEGA OKSIDA

Dvostopenjski proces z raztopino sečnine pri nizki temperaturi je bil uporabljen za pripravo baker/cinkovega oksida. Sferični delci velikosti 5 μm so omogočili nadaljnje izločanje bakra in cinka.

- PODBRŠČEK, Peter, CRNJAK OREL, Zorica, MAČEK, Jadran. Low temperature synthesis of porous copper/zinc oxide. *Mater. res. bull.* [Print ed.], 2009, vol. 44, no. 8, str. 1642–1646. [COBISS.SI-ID 4156186]

## SINTEZA IN STRUKTURNA PODOBNOST ITRIJEVIH IN LANTANOVIH KOMPLEKSNIH KLORIDOV

Mononuklearni molekulski kompleksi , [YCl3(diglyme)(THF)] in [LuCl3 (diglyme)(H2O)], [ErBr3(diglyme)(H2O)], in binuklearni molekulski kompleksi [MCl3 (diglyme)](M = Y , Lu) so bili sintetizirani. Določena je bila koordinacija posameznih centralnih atomov.

- PETRIČEK, Saša. Synthesis and structural similarities of yttrium and lanthanide chloride complexes with diglyme and tetrahydrofuran. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 2, str. 426–433. [COBISS.SI-ID 30530565]

### KRISTALNA STRUKTURA ZSM-12 Z TETRAETILAMONIJEVIMI KATIONI

ZSM-12 z tetraetilamonijevimi kationi je bil sintetiziran in kristalna struktura je bila določena z rentgensko praškovno metodo. To je prva struktura zeolita, v katerem je bila nedvomno določena lega TEA kationa.

- KASUNIČ, Marta, LEGIŠA, Jure, MEDEN, Anton, ZABUKOVEC LOGAR, Nataša, BEALE, Andrew M., GOLOBIČ, Amalija. Crystal structure of pure-silica ZSM-12 with tetraethylammonium cations from x-ray powder diffraction data. *Microporous and mesoporous materials*, 2009, vol. 122, no. 1/3, str. 255–263. [COBISS.SI-ID 30382341]

## DRUGI RELEVANTNI DOSEŽKI

### 1. IZBOLJŠANJE OBSTOJEČEGA TEHNOLOŠKEGA PROCESA OZ. TEHNOLOGIJE

Skupina raziskovalcev programske skupine sodeluje z Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika pri izboljševanju praktične sinteze in proizvodnje različnih produktov, ki jih v Unichemu pripravljajo za prodajo.

### 2. EUROPEAN UNIVERSITY ASSOCIATION- EVALUATION EXPERT POOL

I. Leban je član ekspertnega poola za institucionalno evalvacijo evropskih univerz. V letih 2008 in 2009 je bil član treh evalvacijskih komisij:

- Scitovski, R., Leban, I., Music, S., Rimac, J., Tomas, S.: Završno izvješće o vrednovanju Kemijsko-tehnološkog fakulteta Sveučilišta u Splitu, 2008, 10 str.
- Scitovski, R., Klarić, I., Kronja, O., Leban, I., Šurjak, J.: Završno izvješće o vrednovanju Fakulteta kemijskog inženjerstva i tehnologije Sveučilišta u Zagrebu, 2009, 10 str.
- Amaral, A., Rovio-Johansson, A., D'Ingiana, F., Leban, I., Whelan, N.: Izmir University of Economics, Turkey, EUA evaluation review report, 2009, 24 str.

### 3. ZNANSTVENI PROGRAMSKI ODBOR EPDIC 12

Član programske skupine A. Meden je član Evropskega sveta za praškovno difrakcijo in sodeluje v znanstvenem programskem svetu pri organizaciji 12. evropske konference o praškovni difrakciji (EPDIC 12, Darmstadt, Germany, August 2010).

### 4. ORGANIZACIJA IN PREDSEDOVANJE NA SLOVENSKO-HRVAŠKIH KRISTALOGRAFSKIH SREČANJIH

I. Leban je dolgoletni kopredsednik regionalnih letnih znanstvenih kristalografskih srečanj z mednarodno udeležbo.

2009 18th Croatian-Slovenian Crystallographic Meeting, Varaždin, Hrvatska

Na srečanjih je v povprečju prisotnih med 60 in 80 kristalografov.

## 5. 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 (I. Turel)
- Bilateralno sodelovanje s Srbijo (2008–2009): Struktura in mikrostruktura oksidnih nanomaterialov (A. Meden)

## 6. 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)

## 7. PROMOCIJA ZNANOSTI

- Noč znanstvenic in znanstvenikov 2009 (A. Knez, V. Francetič, I. Leban) http://abra.fkkt.uni-lj.si/fn01leban/rn2009/
- Veselje do znanosti – prikaz poskusov, Gimnazija Celje–Center (A. Knez, I. Leban)

# RESEARCH PROGRAMME REPORT

## PROGRAMME GOALS

Our research programme is divided into fundamental research and applied research and focuses on studies of various new compounds: inorganic, coordination and organometallic. Chemically pure products will be characterized by various physico-chemical methods and also some biological activities will be tested. Similar procedures will be used with new materials. The whole research programme is strongly 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.

## RESEARCH TOPICS

There are several fields of interest within the programme group:

**Quinolones**. Recently, quinolones have been recognized as clinically most successful synthetic antibacterial agents and one of the famous members of this large family-ciprofloxacin (cfH) is a “real blockbuster drug”. Our aim is to prepare novel metal-quinolone complexes and study their physico-chemical properties. One of the goals of the project is to study the interactions of quinolones with biologically active triazoles.

**Complexes of lanthanide halides.** Lanthanides continue to attract interest in science and technology, leading to traditional and new applications. Lanthanides are also used in luminescence, in NMR spectroscopy and in organic synthesis. Complexes of lanthanide chlorides and iodides were intensively studied in the past due to their solubility and reactivity which make them very useful starting compounds. Complexes of lanthanide halides, prevailingly less studied bromides, with simple O- and N-donor ligands will be prepared from lanthanide oxides and lanthanide halides hydrates.

**Discrete organometallic fluorides.** Organotitanium fluorides in their neutral form were found to be catalytically active for polymerization reactions (e.g. for stereospecific polystyrene production). We will focus our research on Ti, Zr, Hf in lanthanoide cyclooctatetraenil (COT) chlorides and fluorides, since catalytic activity is highly expected. In the first step synthesis work and X-ray structural analysis will be performed. Subsequently the most interesting examples will be selected for variable temperature studies with $^{19}$F NMR spectroscopy in the solution.

**Supramolecular self-assembly and host–guest complexation: the case of organotitanium fluorides.** The influence of hydrogen bonding on crystal architecture will be explored. Hydrogen bonds of the type M–F···H–N are strong hydrogen bonds that have been scarcely investigated in fluorochemistry. Special interest will be devoted to non-classical, weak hydrogen bonding of the type M–F···H–C (with $CH_2Cl_2$, $CHCl_3$ …), which present a new and attractive field in supramolecular chemistry.

**Wood protection agents.** Wood protecting agents have been widely commercially used in large quantities for many decades. Due to their bio-toxicity and to preventing of leaching from the wood surface these formulations contain highly toxic chromium and arsenic additives. Environmentally most polluting additives will probably soon be banned. Therefore, a new generation of wood protecting formulations need to be developed. We are planning to search for more adequate formulations for wood protection, with special emphasis on stronger bonding/weaker leaching on/from the protected wood surface.

**Structural work.** Further developments on structural science will be conducted – methodologically as well as theoretically. On the one hand this is driven by the need to structurally characterize novel materials that will be synthesized in the proposed program, and on the other, it is also necessary to follow up and develop the knowledge on structure-properties relationships. The body of knowledge has grown fast in the last years as it is of vital importance for planning materials with desired properties as well as targeted changes. Combination of the powder crystallography and quantum chemical calculations is relatively new, but rapidly developing. As we have kept up with the world scientific achievements in this field we would like to further develop and apply these two methods for simultaneous use in structural elucidation of microwave ceramics, where the results are expected to be very interesting.

**New materials.** Recent developments of the most dynamic areas of science and economy require fast response furnished with research activities and development of new materials with a broad range of properties and applications.

The synthesis and preparation of new materials has been in the forefront of many research programmes. Unrestrained development of diverse methods for their preparation is nowadays replaced by a more deliberate method that takes into consideration factors such as: availability of raw materials with appropriate price, availability of equipment, possibilities for scaling up the process to low tonnage one or even above this level, environmental compatibility of the method, criteria of economic successfulness of the method or process after scaling it up to larger capacities.

The selection of new materials and their combinations in the case of composite materials is directed to the study of catalysts and electro-catalysts. The increasing integration of catalysts into chemical processes in the field of production of diverse chemicals, modern and alternate sources of electrical energy production, and preservation of the environment are guiding us in this direction.

## SCIENTIFIC ACHIEVEMENTS

The following achievements need to be highlighted:

### ORDER/DISORDER OF OXYGEN ANIONS

Successful Rietveld refinements of seven compounds with the formulae $La_2Ti_{(1-x)}Ga_xO_{(5-x/2)}$, where $x = 0.00, 0.20, 0.50, 0.70, 0.90, 0.95$ and $1.00$, were performed in order to describe the solid solubility between $La_2TiO_5$ and $La_4Ga_2O_9$. The similarity of both structures was also described.

– KASUNIČ, Marta, MEDEN, Anton, ŠKAPIN, Srečo D., SUVOROV, Danilo, GOLOBIČ, Amalija. Order-disorder of oxygen anions and vacancies in solid solutions of La[sub]2TiO[sub]5 and La[sub]4Ga[sub]2O[sub]9. *Acta crystallogr., B Struct. sci.*, 2009, vol. B65, no. 5, str. 558–566. [COBISS.SI-ID 30821637]

### MAGNETIC COUPLING OF COPPER(II) IONS

A new hydrogen-bonded dinuclear copper(II) coordination compound has been synthesized from the Schiff-base ligand. Temperature-dependent magnetic susceptibility measurements down to 3 K show that the two metal ions are antiferromagnetically coupled. Strong hydrogen bonding interaction has been clearly evidenced by theoretical calculations.

– TANG, Jinkui, COSTA, José Sánchez, GOLOBIČ, Amalija, KOZLEVČAR, Bojan, ROBERTAZZI, Arturo, VARGIU, Attilio V., GAMEZ, Patrick, REEDIJK, Jan. Magnetic coupling between copper(II) ions mediated by hydrogen-bonded (neutral) water molecules. *Inorg. chem.*, 2009, vol. 48, no. 12, str. 5473–5479. [COBISS.SI-ID 30579205]

### COPPER(II) COORDINATION POLYMERS

The synthesis, structural chemistry and magnetic properties of a series of new Cu(II) polymers with dicarboxylic acids are described. Compounds exhibit either linear chains, whereas others exhibit two-dimensional structure.

– LAH, Nina, CLÉRAC, Rodolphe. Cu(II) coordination polymers incorporating 3-aminopyridine and flexible aliphatic dicarboxylate ligands : synthesis, structure and magnetic properties. *Polyhedron*. [Print ed.], 2009, vol. 28, no. 12, str. 2466–2472. [COBISS.SI-ID 30716165]

### COPPER(II) COMPLEXES WITH SMALL METHANOATE LIGANDS

Copper(II) methanoato complexes may be mononuclear, binuclear or polynuclear. Their properties were determined by various physico-chemical methods.

– KOZLEVČAR, Bojan, MATE, Elizabeta, JAGLIČIĆ, Zvonko, GLAŽAR, Lea, GOLOBIČ, Amalija, STRAUCH, Peter, MONCOL, Jan, KITANOVSKI, Nives, ŠEGEDIN, Primož. A small methanoato ligand in the structural differentiation of copper(II) complexes. *Polyhedron*. [Print ed.], 2009, vol. 28, no. 13, str. 2759–2765. [COBISS.SI-ID 30678021]

### LOW TEMPERATURE SYNTHESIS OF COPPER/ZINC OXIDE

A two-step urea aqueous solution process at a low temperature (90 degrees C) was employed for the preparation of a copper/zinc oxide material. Well defined porous spherical particles with average sizes of around 5 µm in diameter were prepared first and then used as a support for further copper-zinc precipitation

– PODBRŠČEK, Peter, CRNJAK OREL, Zorica, MAČEK, Jadran. Low temperature synthesis of porous copper/zinc oxide. *Mater. res. bull.* [Print ed.], 2009, vol. 44, no. 8, str. 1642–1646. [COBISS.SI-ID 4156186]

### SYNTHESIS AND STRUCTURAL SIMILARITIES OF YTTRIUM AND LANTHANIDE CHLORIDE COMPLEXES

Mononuclear molecular complexes [YCl3(diglyme)(THF)] and [LuCl3 (diglyme)(H2O)], [ErBr3(diglyme)(H2O)], and binuclear molecular complexes [MCl3 (diglyme)](M = Y , Lu) were synthetised.

– PETRIČEK, Saša. Synthesis and structural similarities of yttrium and lanthanide chloride complexes with diglyme and tetrahydrofuran. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 2, str. 426–433. [COBISS.SI-ID 30530565]

### CRYSTAL STRUCTURE OF ZSM-12 WITH TEA CATIONS

Pure-silica ZSM-12 containing tetraethylammonium cations (TEA) was synthesized and its structure was determined from X-ray powder diffraction data. This is the first known zeolite structure in which positions of the TEA cations have been established.

– KASUNIČ, Marta, LEGIŠA, Jure, MEDEN, Anton, ZABUKOVEC LOGAR, Nataša, BEALE, Andrew M., GOLOBIČ, Amalija. Crystal structure of pure-silica ZSM-12 with tetraethylammonium cations from x-ray powder diffraction data. *Microporous and mesoporous materials*, 2009, vol. 122, no. 1/3, str. 255–263. [COBISS.SI-ID 30382341]

## OTHER RELEVANT ACHIEVEMENTS

### 1. IMPROVEMENT OF A TECHNOLOGICAL PROCESS

Collaboration exists with the company Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika. The purpose is to improve the synthesis and the production of new products for the market.

### 2. EUROPEAN UNIVERSITY ASSOCIATION – EVALUATION EXPERT POOL

I. Leban is a member of the pool for the institutional evaluation of European universities. In the years 2008 and 2009 he participated in three evaluations:

– Scitovski, R., Leban, I., Musić, S., Rimac, J., Tomas, S.: Faculty of Chemistry and Technology, University of Split, Final evaluation report, 2008, 10 pp.

– Scitovski, R., Klarić, I., Kronja, O., Leban, I., Šurjak, J.: Faculty of Chemical Engineering and Technology, University of Zagreb, Final evaluation report, 2009, 10pp.

– Amaral, A., Rovio-Johansson, A., D’Ingiana, F., Leban, I., Whelan, N.: Izmir University of Economics, Turkey, EUA evaluation review report, 2009, 24 pp.

## 3. SCIENTIFIC PROGRAMME COMMITTEE FOR EPDIC-12

A. Meden is a member of the European Powder Diffraction Committee and was acting as a member of the Scientific programme committee of the 12th European Powder Diffraction Conference (EPDIC-12, Darmstadt, Germany, August 2010).

## 4. SLOVENIAN-CROATIAN CRYSTALLOGRAPHIC MEETINGS

I. Leban is a co-chairman of regional annual scientific meetings with the international participation.

2009 18th Croatian-Slovenian Crystallographic Meeting, Varaždin, Croatia

The audience is usually between 60 and 80.

## 5. 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)
- Bilateral cooperation with Serbia (2008–2009): Structure and microstructure of oxyde nanomaterials (Principal researcher: A. Meden)

## 6. OTHER COOPERATIONS

- 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)

## 7. PROMOTION OF SCIENCE

- Researchers Night 2009 (A. Knez, V. Francetič, I. Leban)
  http://abra.fkkt.uni-lj.si/fn01leban/rn2009/
- Enjoying Science – experiment show, High School Celje (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**

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# POROČILO O REALIZACIJI PROGRAMA

## CILJI PROGRAMA

1. a) Sinteza novih reagentov na osnovi 3-dimetilaminopropenoatov in sorodnih enaminonov
   b) Aplikacija teh spojin na sintezo novih heterocikličnih sistemov
2. Sinteza naravnih spojin in njihovih analogov z enaminonsko metodologijo
3. Sinteza in transformacije kiralnih spojin
4. Kombinatorna in paralelna sinteza

## OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

Glede na zastavljene cilje je raziskovalno delo potekalo 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

### 1. NOVE METODE ZA SINTEZO FUNKCIONALIZIRANIH HETEROCIKLIČNIH SPOJIN

Študirali smo 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.

1,3-Dipolarne cikloadicije racemnih (1*Z*,4*R**,*R**)-arilmetiliden-4-benzamido-5-fenil-3-pirazolidinon-1-azometiniminov na enatio čisti di-(-)mentil maleat dajo zmesi diastereoizomernih cikloaduktov. Selektivnost in stereokemija cikloadicij sta odvisni od skupin vezanih na 1’-Ar skupini dipola. Pri reakcijah, kjer je vezana vsaj ena ena skupina na orto mestu, nastanejo ali di-(-)-mentil (1*R**,2*S**,3*R**,5*R**,6*R**)-3-aril-6-benzamido-7-okso-5-fenilheksahidropirazolo[1,2-*a*]pirazol-1,2-dikarboksilati in/ali (1*S**,2*R**,3*S**,5 *R**,6*R**)-3-aril-6-benzamido-7-okso-

5-fenillheksahidro pirazolo[1,2-*a*]pirazol-1,2-dikarboksilati s *sin*-orientiranima atomona 3-H in 5-H, medtem ko nastanejo pri orto, orto disubstituiranih spojinah 1*S**,2*R**,3*S**,5 *R**,6*R**)-3-aril-6-benzamido-7-okso-5-fenillheksahidro pirazolo[1,2-*a*]pirazol-1,2-dicarboksilati z *anti*-orientiranima atomoma 3-H in 5-H. (Pezdirc L.; Bevk D.; Pirc S.; Svete J.; *Acta Chim. Slov.* 2009, *56* 545–558) (*OK3*).

V zvezi s sintezo funkcionaliziranih heterociklov velja izpostaviti naslednje dosežke:

Pri regioselektivnih cikloadicijah kiralnih pirazolidin-3-on-1-azometiniminov na etil propiolat na stanejo v prisotnosti Cu(I)I kot katalizatorja cikloadukti, derivati 11,5,6,7-tetrahidropirazolo[1,2-*a*]pirazol-2-karboksilata kot edine regioizomerne spojine. Ugotovili smo, da je stereoselektivnost cikloadicije katalizirane s Cu(I)I odvisna od fenilne skupine na položaju 5 in od skupin vezanih na orto mestih 1'-arilne skupine. (Pezdirc L.; Stanovnik B.; Svete J.; *Aust. J. Chem.* 2009**,** *62*, 1661–1666) (*OK9*).

Razvili smo sedemstopenjsko sintezo 1-substituiranih 5-(2-acilaminoetil)-1*H*-pirazol-4-karboksamidov kot pirazolovih analogov histamina. Sintezo smo začeli najprej s tristopenjsko sinezo $N_1$- substituiranih metil 5-(2-*tert*-butoksikarbonilaminoetil)-1*H*-pirazol-4-karboksilatov iz komercialno dosegljivega Boc-β-alanina. Nato je sledila štiristopenjska pretvorba tega intermediata z acidolitično odstranitvijo Boc skupine, hidrolizo estrske skupine, amidiranjem karboksilne skupine in aciliranjem aminske skupine. Stuktura končnih spojin je bila določena s spektroskopskimi metodami in rentgensko analizo. (Kralj D.; Friedrich M.; Grošelj U.; Kyraly Potpara S.; Meden A.; Wagger J.; Dahmann G.; Stanovnik B., Svete J.; *Tetrahedron* 2009, *65*, 7151–7162) (*OK48*).

Izdelali smo tudi enostavno sintezo 1-substituiranih dietil pirol-3,4-dicarboksilatov iz 2,3-bis-[(*E,E*)-(dimetilamino)metiliden]sukcinatov in aliftskih, aromatskih in heteroaromatskih aminov. Konfiguracijo dvojne vezi C=C smo določili z $^1$H NMR in HMBC spektroskopskimi metodami. (Škrlep L.; Čerček-Hočevar A.; Jakše R.; Stanovnik B.; Svete J.; *Z. Naturforsch., B J. Chem. Sci.* 2009, *64b*, 683–688) (*OK51*).

## 2. NOVE METODE IN REAGENTI V STEREOSELEKTIVNI IN ASIMETRIČNI SINTEZI

Metil (*Z*)-2-(benzoilamino)-3-(dimetilamino)propenoat reagira z trimetilenmetanom. Pri tem nastane metil (*Z*)-2-[benzoil-(2-metilalil)amino]-3-(dimetilamino)propenoat, ki smo ga nato pretvorili v derivate pirazola s postopnimi reakcijami: izmenjavo dimetilaminske skupine s hidazinom in ciklizacijo z estrsko skupino. Pri reakciji pirazolov z 1,2,4,5-tetrazin-3,6-dikarboksilatom nastanejo diastereoizomerni 1-aril-6'-benzoil-4a'-metil-5-okso-1,4',4'a,5,5',6'-heksahidrospiro-[pirazol-4,7'-pirolo[3,4-*c*]piridazin]-3',7a'(1'*H*)-dikarboksilati. Ta pretvorba predstavlja enostavno pot so novih heterocikličnih sistemov. (Uršič U.; Grošelj U.; Meden A.; Svete J.; Stanovnik B.; *Synthesis* 2009, 217-226) (*OK43*).

Študirali smo[2+2] cikloadicije 2-amino-3-dimetilaminopropenoatov z acetilenkarboksilati pod vplivom mikrovalov. Pri tem so nastali polifunkcionalizirani derivati 1-amino-4-(dimetilamino)buta-1,3-dienov. Pri vseh reakcijah je nastala samo ena izomerna oblika in tudi pri nesimetrično substituiranih acetilenih je reakcija potekala regiospecifično. V nadaljevanju smo študirali [2+2] cikloadicije acetilen mono in dikarboksilatov na (5*Z*)-5-[(dimetilamino) metilen]imidazolidin-2,4-dione in na ustrezne tiookso derivate pod vplivom mikrovalov. Pri tem so nastali v acatonitrilu polifunkcionalno substituirani derivati imidazolidin-2,4-dionov, v DMF pa je potekla delna hidroliza do polisubstituiranih butandioatov. (Uršič U.; Grošelj U.; Meden A.; Svete J.; Stanovnik B.; *Helv. Chim. Acta* 2009, *92*, 481–490) (*OK22*).

## 3. KOMBINATORNA SINTEZA HETEROCIKLIČNIH SPOJIN

Zgoraj omenjene študije na področju heterociklične sinteze smo nadgradili tudi z naslednjimi aplikacijami v kombinatorni sintezi.

Izdelali smo dve varianti paralelne sinteze v raztopini N-substituiranih dimetil 4-okso-1,4-dihidropiridin-3,5-dikarboksilatov in metil 3-okso-3,5-dihidro-2*H*-pirazolo[4,3-*c*]piridin-7-karboksilatov iz aceton-1,3-dikarboksilatov. Po prvi varianti smo najprej pripravili bisenaminonski reagent iz 1,3-acetondikarboksilata, pri drugi varianti pa smo izhajali iz mono enaminonskega reagenta pripravljenega iz aceton-1,3-dikarboksilata. Nato smo izmenjevali dimetilamisko skupino s primarnimi amini in tako nastale intermediate ciklizirali v dihidropirindikarboksilate. (Baškovč J.; Bevk D.; Stanovnik B.; Svete J.; *J. Comb. Chem.* 2009, *11,* 500–507) (*OK29*).

## 4. SINTEZA NOVIH HETEROCIKLIČNIH SISTEMOV

Iz dietil aceton-1,3-dikarboksilata smo pripravili 2-amino-4-(2-etoksi-2-oksoetil)tiazol-5-karboksilat, ki smo ga nato pretvorili z dimetilformamid dimetilacetalom (DMFDMA) v ustrezni dimetilaminometilidenamino derivate, iz katerih nastanejo pri substituciji s primarnimi amini in sledečo ciklizacijo 6-substituirani derivati 2-aminotiazolo[5,4-*c*]piridin-4-karboksilata, s hidrazini pa 6-amino substituirani 2-aminotiazolo[5,4-c]piridin-4-karboksiati. (Albreht A.; Uršič U.; Svete J.; Stanovnik B.; *Heterocycles* 2009, *78*, 2343–2352) (*OK26*).

Dietil 2-[(dimetilamino)metilen]-3-oksopentandioate, ki smo jih pripravili iz dietil aceton-1,3-dikarboksilata in DMFDMA, smo direktno pretvorili z gvanidin hidrokloridom v etil 2-amino-4-(2-etoksikarbonilmetil)pirimidin-5-karboksilat in etil 4-[1-(dimetilamino)-3-etoksi-3-oksoprop-1-en-2-yl]-2-[(dimetilamino)metilenamino]pirimidin-5-karboksilat. Iz zadnjega smo pri reakciji z amoniakom, primarnimi amini, hidrazinom an hidroksilaminom pripavili 6-substituirane 2-amino-5-okso-5,6-dihidropirido[4,3-*d*]piridin-8-karboksilate. (Zupančič S.; Svete J.: Stanovnik B.; *Heterocycles* 2009**,** *77*, 899-908) (*OK25*).

Podobno smo iz dimetil aceton-1,3-dikarboksilata, sulfuril klorida in tiosečnine pripravili metil 2-amino-4-(2-metoksi-2-oksoetil)tiazol-5-karboksilat, ki smo ga nato v dveh stopnjah pretvorili v derivate (4*H*-pirido[1,2-*a*]pirimidin-3-il)tiazol-5-karboksilata. (Žugelj M.; Albreht A.; Uršič U.; Svete J.; Stanovnik B.; *ARKIVOC* 2009, No.VI, 137–145) (*OK8*).

## 5. SODELOVANJE Z DRUGIMI UNIVERZAMI

V sodelovanju z univerzo v Bydgoszczu (Poljska) smo študirali vpliv vinilenskih in 1,4-fenilenskih distančnikov na osnovno stanje pri intramolekularnem prenosu naboja pri 4-dimetilamino-1-metilpiridinijevih kationih. (Gawinecki R.; Stanovnik B.; Valkonen A.; Kolehmainen E.; Osmiałowsky B.; Dobosz R.; Zakrzewska A.; *Struct. Chem.* 2009, *20*, 655–662) (*OK38*).

V sodelovanju z ETH v Zürichu je dr. Uroš Grošelj kot postdoktorand pri prof. D. Seebachu v šolskem letu 2008/2009 opravil naslednje delo:

Dandanes je asimetrična organokataliza prepoznana, poleg že uveljavljenih organokovinskih in bioloških pristopov k asimetrični katalizi, kot učinkovita in zanesljiva tretja strategija pri stereoselektivni pripravi pomembnih kiralnih spojin. Med množico objav s področja organokatalize lahko najdemo le peščico objav, ki obravnavajo mehanistične aspekte organokatalize. Naš članek opisuje in detajlno analizira do sedaj prvo izolacijo in strukturno karakterizacijo reaktivnih intermediatov v organokatalizi z derivati difenil-prolinola in imidazolidinona. Tako smo pri reakciji 2-fenilacetaldehida z $Me_3Si$ etrom difenil-prolinola, z odstranitvijo vode, izolirali ustrezen enamin. Pri reakciji $HBF_4$ soli $MePh_2Si$ etra difenil-prolinola in 2-(*terc*-butil)-3-metil in 5-benzil-2,2,3-trimetil-1,3-imidazolidin-4-ona s cinamaldehidom smo izolirali ustrezne iminijeve soli. Z rentgenskimi strukturnimi podatki enega enamina in dveh iminijevih soli ter z NMR analizami smo potrdili splošno sprejeti strukturi dveh tipov reaktivnih intermediatov v organokatalizi s petčlenskimi heterocikli, to je enamine in iminijeve soli. Fine detajle rentgenskih struktur smo analizirali s stališča opaženih stereoselektivnosti pri ustreznih reakcijah z elektrofili in nukleofili. Strukture reaktivnih intermediatov pripravljenih iz diarilprolinol etrov smo primerjali z ostalimi difenil-prolinolnimi derivati (rentgenske strukture iz Cambridge File CSD) in jih analizirali v povezavi z ostalimi reagenti in ligandi, ki vsebujejo geminalne diarilne skupine in se jih uporablja v stereoselektivni sintezi. Iminijeve ione smo primerjali tudi z *N*-aciliranimi imidazolidinoni in analizirali skupne strukturne aspekte, kot so minimizacija 1,5-odbojev ($A^{(1,3)}$ efekt). Poleg tega smo kristalne strukture primerjali s predhodno objavljenimi teoretičnimi strukturami, dobljenimi z DFT-izračuni na visokem nivoju teorije. Fine podrobnosti, vključujoč piramidalizacijo na trigonalnem *N*-atomu, zvitje C=N vezi, ščitenje diastereotopnih strani in π-interakcije med benzenovim obročem in Me skupino, se tako dobro ujemajo s teoretskimi izračuni, ki so praktično predvideli eksperimentalne rezultate, da se je smiselno vprašati, ali bomo kmalu v prihodnosti najprej izvedli take izračune, preden se bomo podali v laboratorij optimizirati eksperiment. (Seebach D.; Grošelj U.; Badine D. M.; Schweizer W. B.; Beck A. K.; *Helv. Chim. Acta* 2008, *91*, 1999–2034) (*OK52*).

V naslednjem članku je opisana izolacija in strukturna karakterizacija reaktivnih intermediatov v organokatalizi s prvo in drugo generacijo uveljavljenih komercialno dostopnih *MacMillanovih* imidazolidinonskih katalizatorjev in nekaterih drugih imidazolidinonskih iminijevih intermediatov, pospremljena s poglobljeno diskusijo. Objavljene so tri rentgenske strukture (*E*)-1-cinamoiliden iminijevih $PF_6$ soli in sicer 5-benzil-2,2,3-trimetilimidazolidin-4-ona (*MacMillanov* katalizator prve generacije), *cis*-5-benzil-2-*terc*-butil-3-metilimidazolidin-4-ona (*MacMillanov* katalizator druge generacije), in *cis*/*trans*-5-benzil-2-stiril-3-metilimidazolidin-4-ona. Pri 2,2-dimetil in pri *cis*-2-stiril derivatu smo opazili, da je vez C-H na položaju 2 usmerjena v sredino benzenovega obroča benzilne skupine, ki leži nad petčlenskim obročem. NMR meritve kažejo na to, da je ista struktura/konformacija prisotna tudi v raztopini. Pri *cis*-2-(*terc*-butil) derivatu pa je benzilna skupina locirana nad iminijevim π-sistemom. Prekrivanje z DFT-izračunanimi krotonilidenskimi analogi kaže skoraj popolno superimpozicijo teoretičnih in eksperimentalno izmerjenih struktur. Strukture v članku obravnavamo s stališča njihovih vlog kot reaktivnih intermediatov v organokatalizi in s stališča pomoči, ki jo sintezni organski kemik lahko črpa iz teorije. (Grošelj U.; Schweizer W. B.; Ebert M.- O.; Seebach D.; *Helv. Chim. Acta* 2009, *92*, 1–13) (*OK21*).

Določili smo večje število struktur reakcijskih intermediatov (enaminov in iminijevih ionov) v organokatalizi z metilnimi in sililnimi etri diarilprolinola (večina le-teh je uveljavljenih komercialno dostopnih katalizatorjev, npr. *Jørgensenov* 2-[bis(3,5-bistrifluorometilfenil)trimetilsilaniloksimetil]pirolidin katalizator). Reakcijske intermediate smo sintetizirali/izolirali in v celoti okarakterizirali. Pripravili smo iminijeve soli z $BF_4$, $PF_6$, $SbF_6$, in šibko koordinirajočim $Al[OC(CF_3)_3]_4$ anionom. Dobili smo rentgenske strukture enega enamina in šestih iminijevih soli, katerih strukture so opisane v tem članku in v predhodni komunikaciji (*Helv. Chim. Act*a 2008, *91*, 1999). Sodeč po NMR spektrih (v $CDCl_3$, ($D_6$)DMSO, ($D_6$)aceton ali $CD_3OD$) ima večinski izomer iminijevih soli (*E*)-konfiguracijo okoli N=C(1') vezi, poleg tega pa je v raztopini prisoten tudi (*Z*)-izomer in sicer do 11 %. V vseh rentgenskih strukturah ima iminijev ion (*E*)-konfiguracijo, konformacija okoli eksociklične N-C-C-O vezi pa je sinklinalna-*ekso*, z eno od fenilnih skupin nad pirolidinskim obročem, in RO-skupino nad π-sistemom. Prav tako je eden od *meta*-substituentov (Me ali $CF_3$) 3,5-disubstituirane fenilne skupine pozicioniran v prostoru nad π-sistemom. DFT izračuni na različnih nivojih teorije potrjujejo, da so eksperimentalno določene strukture daleč najstabilnejše (do 8.3 kcal/mol). Diskusija v članku vključuje eksperimentalno določene rezultate v povezavi z mehanizmom v organokatalizi z derivati diarilprolinola kot katalizatorji. (Grošelj U.; Seebach D.; Badine D. M.; Schweizer W. B.; Beck A. K.; Krossing I.; Klose P.; Hayashi Y.; Uchimaru T.; *Helv. Chim. Acta* 2009, *92*, 1225–1259) (*OK24*).

## 6. PREGLEDNI ZNANSTVENI ČLANKI

- STANOVNIK, Branko. Alkyl 3-(dimethylamino)propenoates and related enaminones in the synthesis of heterocyclic systems. V: EDER, Maria (Ed.). *20. Jahre Europäische Akademie der Wissenschaften und Künste : Festschrift*, (Edition Weimar, Book series of European Academy of Sciences and Arts, Vol. 13). Weimar: VDG, Verlag und Datenbank für Geisteswissenschaften, 2009, pp. 247–269. (*OK76*).
- WAGGER, Jernej, KRALJ, David, SVETE, Jurij, STANOVNIK, Branko. Ethyl isothiocyanatoacetate. V: PAQUETTE, Leo A. (Ed.). *Encyclopedia of reagents for organic synthesis*. 2nd ed. Chichester: J. Wiley and Sons, 2009, pp. 4966–4969. (*OK72*).
- SEEBACH, Dieter, BECK, Albert K., CAPONE, Stefania, DENIAU, Gildas, GROŠELJ, Uroš, ZASS, Engelbert. Enantioselective preparation of [beta][sup]2-amino acid derivatives for [beta]-peptide synthesis. *Synthesis (Stuttg.)*, 2009, no. 1, pp. 1–32. (*OK56*).

β-Amino kisline z eno samo stransko verigo na α-položaju ($\beta^2$-amino kisline ali H-$\beta^2$hXaa(PG)-OH; *i.e.*, homo-amino kisline s proteinogenimi stranskimi skupinami) so se izkazale za pomembne gradnike β-peptidov. β-Amino kisline v β-peptidih so odgovorne za tvorbo edinstvenih sekundarnih struktur, so potrebne za oponašanje strukture in aktivnosti α-peptidov, ki tvorijo β-zavoje in lahko jih uporabimo za zaščito α-peptidov proti napadu aminopeptidaz. Za razliko od $\beta^3$-homo-amino kislin, $\beta^2$-izomerov ne moremo pripraviti s preprosto enantiospecifično homologacijo (naravnih) α-amino kislin, ampak jih moramo pripraviti z enantioselektivnimi reakcijami ali sekvencami pretvorb, ki so opisane v tem preglednem članku. Različne sintezne metode so razdeljene glede na vez na stereogenem centru, ki se tvori v stereoselektivnem koraku. Te štiri strateške vezi na stereogenem centru so: C(2)–C(3) vez ogrodja, vez C(2)-stranska veriga, vez C(2)–H in vez C(1)–C(2) med karboksilatom in α-C atomom. Pri najpogosteje uporabljenih sinteznih poteh je na karboksilnem C(1) atomu ali na dušiku na mestu 3 vezano kiralno pomagalo, poleg teh pa je znana še množica enantioselektivnih katalitskih procesov, vključujoč hidrogeniranja ustreznih akrilatov. Članek obravnava tudi alternative stereoselektivni sintezi, in sicer ločevanje racemnih zmesi (npr. z biokatalizo). Predstavljena je kritična primerjava različnih sinteznih metod in strategij. Za peptidnega kemika je priložena lista $\beta^2$-amino kislinskih gradnikov, z Cbz–, Boc– in Fmoc-zaščitnimi skupinami, primernih za tvorbo peptidov. Poleg tega je opisana podrobna strategija iskanja neracemnih $\beta^2$-amino kislin in njihovih prekurzorjev iz baze podatkov.

- SVETE, Jurij. (4R*,5R*)-4-benzoylamino-5-phenyl-3-pyrazolidinone: a useful building block in the synthesis of functionalized pyrazoles. V: HORVAT, Monika A. (Ed.). *Stereochemistry research trends*. New York: Nova Science Publishers, cop. 2008, pp. 129–193, graf. prikazi. (*OK75*).

Pregled kemije (4*R**,5*R**)-4-benzoilamino-5-fenil-3-pirazolidinona(**1**) kot lahko dostopnega in uporablnega gradnika za sintezo funkcionaliziranih pirazolov, ki vsebujejo *α*-amino kislinski ali peptidni strukturni element. Najbolj uporabni derivati pirazolidinona **1** so njegovi stablini azometin imini **2**, ki nastanejo pri reakcijah z aromatskimi aldehidi. V tem kontekstu, je bilo največ pozornosti posvečeno [3+2] cikloadicijam azometin iminov **2**. Dipoli **2** imajo širok spekter reaktivnosti (konektivnosti), pri čemer je večina cikloadicij stereoselektivnih. Visoka stopnja stereoselektivnosti in enostavnost izolacije cikloaduktov omogočata tudi kombinatorno sintezo pirazolo[1,2–*a*]pirazolonskih peptidomimetikov z variabilno amino kislinsko sekvenco ter z variabilno, a predvidljivo konfiguracijo.

## DRUGI RELEVANTNI DOSEŽKI

### A) UREDNIŠTVO

- PEJOVNIK, Stane, STANOVNIK, Branko (Ed.). *90 let kemijskih študijev na Univerzi v Ljubljani: 1919–2009*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2009. 159 pp., ilupp. ISBN 978-961-6756-10-5. (*OK89*).
- 13th Blue Danube Symposium on Heterocyclic Chemistry, Bled, September 20–23 2009, Slovenia, STANOVNIK, Branko (Ed.), SVETE, Jurij (Ed.). *Program. Abstracts of papers. List of participants*. Ljubljana: Organizing Committee, 2009. 163 pp., ilupp. (*OK90*).
- PANICO, Robert (Ed.), POWELL, Warren H. (Ed.), RICHER, Jean-Claude (Ed.), STANOVNIK, Branko (Ed.), TIŠLER, Miha (Ed.). *Vodnik po nomenklaturi organskih spojin IUPAC : priporočila 1993 (vključno s spremembami glede na nomenklaturo organske kemije IUPAC 1979)*. Ponatis izd. iz leta 1999. Ljubljana: Slovenska akademija znanosti in umetnosti, 2009. IX, 185 pp., ilupp. ISBN 978-961-6242-24-0. (*OK91*).
- *Acta chimica slovenica*. Svete, Jurij (gostujoči urednik 2009). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: = Slovenian Chemical Society, 1993–. ISSN 1318–0207. (*OK94*).

### B) PLENARNA IN VABLJENA PREDAVANJA

- STANOVNIK, Branko. [beta]-Dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related enaminones. Versatile reagents for preparation of various heterocyclic systems including natural products : [invited lecture]. V: *The 10th Annual Florida heterocyclic and synthetic conference : march 8th–march 11th, 2009*. [S. l.: s. n.], 2009, pp. 52. (*OK58*).
- WAGGER, Jernej, SVETE, Jurij, STANOVNIK, Branko. 3-Dimethylamino-2-acylamino and related enaminones in the synthesis of natural products : [invited lecture]. V: *9. Tagung Iminiumsalze, 7.–10. September 2009 in Bartholomä/Ostalbkreis, "Sport- und Bildungszentrum Bartholomä" : IMSAT-9*. [S. l.: s. n.], 2009, pp. 30–36. (*OK59*).
- SVETE, Jurij. Enaminones in combinatorial synthesis of heterocycles : [invited lecture]. V: *9. Tagung Iminiumsalze, 7.–10. September 2009 in Bartholomä/Ostalbkreis, "Sport- und Bildungszentrum Bartholomä" : IMSAT-9*. [S. l.: s. n.], 2009, pp. 6–15. (*OK62*).
- STANOVNIK, Branko. [beta]-Dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related enaminones : versatile reagents for preparation of various heterocyclic systems : [plenary lecture]. V: The Transmediterranean Colloquium on Heterocyclic Chemistry, 5–7 November 2009, Laico Hotel, Yasmine Hammamet. *Lectures and communications abstracts participants' list : TRAMECH 6*. [S. l.: s. n.], 2009, pp. Lecture 5. (*OK60*).

- WAGGER, Jernej, GOLIČ GRDADOLNIK, Simona, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. Enaminones in the synthesis of some unsaturated tryptophan ([triangle]Trp) containing alkaloid analogues : [invited Blue Danube lecture]. V: STANOVNIK, Branko (Ed.), SVETE, Jurij (Ed.). 13th Blue Danube Symposium on Heterocyclic Chemistry, Bled, September 20–23, 2009, Slovenia. *Program. Abstracts of papers. List of participants*. Ljubljana: Organizing Committee, 2009, pp. 36. (*OK63*).

## C) PREDAVANJE NA TUJI ZNANSTVENI INSTITUCIJI

- STANOVNIK, Branko. *[beta]-Dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related enaminones – versatile reagents for preparation of various heterocyclic systems including natural products : [Bulgarian Academy of Sciences, Sofia, Bulgaria, 7th April, 2009]*. Sofia, 2009. (*OK82*).

## D) ORGANIZACIJA MEDNARODNEGA KONGRESA

V letu 2009 smo organizirali mednarodni simpozij 13th Blue Danube Symposium on Heterocyclic Chemistry, ki je potekal od 20. do 23. septembra na Bledu. Predsednik Mednarodnega znanstvenega odbora B. Stanovnik, predsednik Organizacijskega odbora B. Stanovnik, podpredsednik Organizacijskega odbora J. Svete.

## E) MEDNARODNO PRIZNANJE

B. Stanovnik:

2009 Plaketa Tunizijskega kemijskega društva, Hammamad, Tunizija.

## F) ČLANSTVO MEDNARODNIH ZNANSTVENIH ODBOROV 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 on Heterocyclic Chemistry
c) Member of the Board of Electron Journal ARKIVOC
d) Member of the Advisory Board "Advances in Heterocyclic Chemistry"
e) Member of the Scientific Committee, TRAMECH, Transmediterranean Symposia of Heterocyclic Chemistry
f) Member of the 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) Predstojnik Oddelka za mednarodno sodelovanje in znanstveno koordinacijo Slovenske akademije znanosti in umetnosti, Ljubljana, Slovenija
j) Dekan razreda za naravoslovne znanosti Evropske akademije znanosti in umetnosti, Salzburg, Avstrija in legat EASA za Slovenijo za obdobje 2010–2014
k) Member of the Advisory Board, Croatica Chemica Acta

l) Member of the Advisory Editorial Board, Journal of Heterocyclic Chemistry

m) 1998–2004 Member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons, Den Haag, The Netherlands

n) Chairman of the Advisory Editorial Board, Vestnik Slovenskega kemijskega društva, (since 1994 Acta Chimica Slovenica) Slovenia

o) Associate Editor, Bull. Soc. Chim. Belges, Belgium

## RESEARCH PROGRAMME REPORT

### PROGRAMME GOALS

1. a) Synthesis of new reagents on the basis of 3-dimethylaminopropenoates and related enaminones
   b) Application of these reagents to the synthesis of new heterocyclic systems
2. Synthesis of natural products and their analogues by enaminone methodology
3. Synthesis and transformation of chiral compounds
4. Combinatorial and parallel synthesis

### RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

The research work was carried out in the following fields:

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

#### 1. NEW METHODS FOR THE SYNTHESIS OF FUNCTIONALIZED HETEROCYCLIC COMPOUNDS

We studied novel synthetic methods and approaches for the preparation of heterocycles functionalized with terpene, ethylamine, amino acid, dipeptide, amino alcohol, and related structural elements. 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 cyclo additions of azomethine imines on various acetylenes and olefins.

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

1,3-Dipolar cyloaddition of racemic (1*Z*,4*R**,*R**)arylmethylidene-4-benzamido-5-phenyll-3-pyrazolidinon-1-azomethinimines to enantiopure di-(-)menthyl maleate afforded mixtures of diastereoisomeric cycloadducts. Selectivity and stereochemistry of cycloadditions were dependent on the substituents at the 1'-Ar residue of dipoles. Reactivity of dipoles with at least one free *ortho*-positon gave either di-(-)-menthyl (1R*,2S*,3R*,5R*,6R*)-3-aryl-6-benzamido-7-oxo-5-phenylhexahydropyrazolo[1,2-*a*]pyrazole-1,2-dicarboxylate and/or (1S*,2R*,3S*,5 R*,6R*)-3-aryl-6-benzamido-7-oxo-5-phenylhexahydro pyrazolo[1,2-*a*]pyrazole-1,2-dicarboxylates with *syn*-oriented 3-H and 5-H, while reactions with *ortho* disubstituted dipoles gave (1S*,2R*,3S*,5 R*,6R*)-3-aryl-6-benzamido-7-oxo-5-phenylhexahydropyrazolo[1,2-*a*]pyrazole-1,2-dicarboxylates with *anti*-oriented 3-H in 5-H. (Pezdirc L.; Bevk D.; Pirc S.; Svete J.; *Acta Chim. Slov.* 2009, *56* 545–558) (*OK3*).

Regiospecific copper(I) iodide catalyzed cycloadditions of chiral pyrazolidin-3-on-1-azomethine imines to ethyl propyolate gave cycloadducts, derivates of 1,5,6,7-tetrahydropyrazolo[1,2-*a*]pyrazole-2-carboxylate as single diastereoismers. Stereoselectivity of copper(I) iodide-catalyzed cycloadditions was controlled by the stereodirecting phenyl group at position 5 and by the *ortho*-substituents at the 1'-aryl residue. (Pezdirc L.; Stanovnik B.; Svete J.; *Aust. J. Chem.* 2009, *62*, 1661–1666) (*OK9*).

A seven-step synthesis of 1-substituted 5-(2-acylaminoethyl)-1*H*-pyrazole-4-carboxamides as pyrazole analogs of histamine was developed. Synthesis starts with a three-step preparation of $N_1$- substituted methyl 5-(2-*tert*-butoxycarbonylaminoethyl)-1*H*-pyrazole-4-carboxylates from commercially available Boc-β-alanine. Subsequent four-step transformation of this intermediate was performed with acidolytic removal of Boc group, hydrolysis of the ester group, amidations of carboxylic group and acylation of amino group. (Kralj D.; Friedrich M.; Grošelj U.; Kyraly Potpara S.; Meden A.; Wagger J.; Dahmann G.; Stanovnik B.; Svete J.; *Tetrahedron* 2009, *65*, 7151–7162) (*OK48*).

A series of 1-substituted diethyl pyrrole-3,4-dicarboxylates by treatment of 2,3-bis-[(*E,E*)-(dimethylamino)methylidene]succinates with aliphatic, aromatic and heteroaromatic amines. Configuration of the C=C double bond was determined by $^1$H NMR and HMBC spectroscopic methods. (Škrlep L.; Čerček-Hočevar A.; Jakše R.; Stanovnik B.; Svete J.; *Z. Naturforsch., B J. Chem. Sci.* 2009, *64b*, 683–688) (*OK51*).

## 2. NEW METHODS AND REAGENTS IN STEREOSELECTIVE AND ASYMMETRIC SYNTHESIS

(*Z*)-Methyl 2-benzamido-3-dimethylaminopropenoate reacted with trimethylenemetane to produce (*Z*)-methyl 3-(dimethylamino)-2-(*N*-(methylallyl)benzamido)propenoate, which was then converted into pyrazole derivatives by a consecutive exchange of the dimethylamino group with hydrazine derivates and cyclisation to the ester group. Reactions of pyrazoles with dimethyl 1,2,4,5-tetrazine-3,6-dicarboxylate resulted in a diasteroeselective formation of 1-aryl-6'-benzoyl-4a'-methyl-5-oxo-1,4',4a',5,5',6',7a'-octahydrospiro[pyrazole-4,7'-pyrrolo[3,4-*c*]pyridazine]-3',7a'-dicarboxylates. This represents a simple new pathway to novel heterocyclic systems. On the other hand, when dimethylaminopropenoate reacted with aniline hydrochloride, followed by the cycloaddition of 1,2,4,5-tetrazine, (*E*)- and (*Z*)-dimethyl 4-((*N*-(3-methoxy-3-oxo-1-(phenylamino)prop-1-en-2-yl)benzamido)-methyl)-4-methyl-1,4-dihydropyridazine-3,6-dicarboxylates were formed respectively. (Uršič U.; Grošelj U.; Meden A.; Svete J.; Stanovnik B.; *Synthesis* 2009, 217–226) (*OK43*).

Microwave-assisted [2+2] cycloadditions of acetylene mono- and dicarboxylates to (*Z*)-5-[(d imethylamino)methylene]imidazolidine-2,4-diones in MeCN furnished highly functionalized imidazolidine-2,4-dione derivatives as single isomers or mixtures of two isomers. When the reaction of (*Z*)-5-[(dimethylamino)methylene]imidazolidine-2,4-dione with acetylenedicarboxylate was performed in DMF, hydrolysis of the (dimethylamino)methylene group took place to give (2*E*)-2-(2,5-dioxoimidazolidin-4-ylidene)succinate. (Uršič U.; Grošelj U.; Meden A.; Svete J.; Stanovnik B.; *Helv. Chim. Acta* 2009, *92*, 481-490) (*OK22*).

## 3. COMBINATORIAL SYNTHESIS OF HETEROCYCLIC COMPOUNDS

The above mentioned studies in the field of heterocyclic synthesis were also extended towards applications in combinatorial synthesis. The following methods were developed:

Two variations of parallel solution-phase synthesis of N-substituted dimethyl 4-oxo-1,4-dihydropyridine-3,5,-dicarboxylates and methyl 3-oxo-3,5-dihydro-2*H*-pyrazolo[4,3-*c*]pyridine-7-carboxylates from acetone-1,3-dicarboxylates were developed. The first synthetic method comprises preparation of bisenaminone reagents and their cyclization with primary amines, while the other method consists of the preparation of monoenaminone reagents followed by substitution of the dimethylamino group with primary amines, followed by cyclization with DMFDMA. (Baškovč J.; Bevk D.; Stanovnik B.; Svete J.; *J. Comb. Chem.* 2009, *11,* 500–507) (*OK29*).

## 4. SYNTHESIS OF NEW HETEROCYCLIC SYSTEMS

Ethyl 4-[1-(dimethylamino)-3-ethoxy-3-oxoprop-1-en-2-yl]-2-[(dimethylamino)methylidene-amino]thiazole-5-carboxylate, prepared by a known procedure from ethyl 2-amino-4-(2-ethoxy-2-oxoethyl)thiazole-5-carboxylate, was transformed with aromatic amines into 5-aryl substituted 2-aminothiazolo[5,4-*c*]pyridine-7-carboxylates, while treatment of with monosubstituted hydrazines produced 5-*N*-amino substituted thiazolo[5,4-*c*]pyridine-7-carboxylates. (Albreht A.; Uršič U.; Svete J.; Stanovnik B.; *Heterocycles* 2009, *78*, 2343–2352) (*OK26*).

Diethyl 2-[(dimethylamino)methylene]-3-oxopentanedioate, prepared from acetone-1,3-dicarboxylates and *N,N*-dimethylformamide dimethylacetal (DMFDMA) was, without isolation, transformed by treatment with guanidine hydrochloride into ethyl 2-amino-4-(2-ethoxy-2-oxoethyl)- pyrimidine-5-carboxylate. This compound was transformed with DMFDMA first into intermediate and with an excess of DMFDMA into ethyl 4-[1-(dimethylamino)-3-ethoxy-3-oxoprop-1-en-2-yl]-2-[(dimethylamino)methyleneamino]pyrimidine-5-carboxylate. By treating the compound with ammonia, primary amines, hydrazine or hydroxylamine, intermediates were formed, which cyclized into 6-substituted 2-amino-5-oxo-5,6-dihydropyrido[4,3-*d*]pyridine-8- carboxylates. (Zupančič S.; Svete J.; Stanovnik B.; *Heterocycles* 2009**,** *77*, 899–908) (*OK25*).

Methyl 2-amino-4-(2-methoxy-2-oxo-ethyl)thiazole-5-carboxylate, prepared from dimethyl acetone-1,3-dicarboxylate, sulfuryl chloride and thiourea according to a known procedure, was transformed in two steps into (4*H*-pyrido[1,2-*a*]pyrimidin-3-yl)thiazole-5-carboxylates. (Žugelj M.; Albreht A.; Uršič U.; Svete J.; Stanovnik B.; *ARKIVOC* 2009, No.VI, 137–145) (*OK8*).

## 5. COOPERATION WITH OTHER UNIVERSITIES

In cooperation with Prof. R. Gawinecki from the University of Bydgoszcz (Poland), the effect of vinylene and 1,4-phenylene spacers on the efficiency of the ground-state intramolecular charge-transfer in enlarged 4-dimethylamino-1-methylpyridinium cations was studied. (Gawinecki R.; Stanovnik B.; Valkonen A.; Kolehmainen E.; Osmiałowsky B.; Dobosz R.; Zakrzewska A.; *Struct. Chem.* 2009, *20*, 655–662) (*OK38*).

Dr. Uroš Grošelj has been a postdoctorate fellow with Prof. Seebach at the ETH in Zürich (Switzerland) in academic year 2008/2009. His research includes the following topic:

Nowadays, asymmetric organocatalysis is recognized, alongside with the established organometallic and biological approaches to asymmetric catalysis, as an efficient and reliable third strategy for the stereoselective preparation of valuable chiral compounds. Among numerous reports in this field only few investigated the mechanistic aspects of organocatalysis. The article describes and discusses in detail the first ever isolated and structurally characterized reactive intermediates in organocatalysis with diphenyl-prolinol and imidazolidinone derivatives. Thus, the reaction of 2-phenylacetaldehyde with the $Me_3Si$ ether of diphenyl-prolinol, with removal of $H_2O$, gave the corresponding enamine. The $HBF_4$ salts of the $MePh_2Si$ ether of diphenyl-prolinol and of 2-(*tert*-butyl)-3-methyl and 5-benzyl-2,2,3-trimethyl-1,3-imidazolidin-4-one reacted with cinnamaldehyde to give the corresponding iminium salts. Single crystals of enamine and of two iminium salts were subjected to X-ray structure analysis and a $^2$D-NMR spectrum of the third iminium salt was recorded. The crystal and NMR structures confirmed the commonly accepted, general structures of the two types of reactive intermediates in organocatalysis with five-membered heterocycles, *i.e*., enamines and iminium salts. Fine details of the crystal structures are discussed in view of the observed stereoselectivities of the corresponding reactions with electrophiles and nucleophiles. The structures of diarylprolinol ether-derived reactive intermediates are compared with those of other diphenyl-prolinol derivatives (from the Cambridge File CSD) and discussed in connection with other reagents and ligands, containing geminal diaryl groups and being used in enantioselective synthesis. The iminium ions are compared with *N*-acylated imidazolidinones, and common structural aspects such as minimalization of 1.5-repilsion (the ‘$A^{(1,3)}$-effect’), are discussed. Finally, the crystal structures are compared with previously published theoretical structures, which were obtained from high-level-of-theory DFT calculations. Delicate details including pyramidalization of trigonal *N*-atoms, distortions around iminium C=N bonds, shielding of diastereotopic faces, and the π-interaction between a benzene ring and a Me group matched well, and were actually predicting the experimental results. Thus a question may be appropriate as to whether we may start considering making such calculations before going to the laboratory for experimental optimizations. (Seebach D.; Grošelj U.; Badine D. M.; Schweizer W. B.; Beck A. K.; *Helv. Chim. Acta*, 2008, *91*, 1999–2034) (*OK52*).

The following article describes and discusses in detail the isolation and structural characterization of reactive intermediates in organocatalysis with *MacMillan's* first and second generation established, commercially available imidazolidinone derived organocatalysts and some other imidazolidinone derived iminium intermediates. Thus, the X-ray crystal structures of three (*E*)-1-cinnamoylidene iminium $PF_6$ salts of 5-benzyl-2,2,3-trimethylimidazolidin-4-one (*MacMillan's* first generation catalyst), *cis*-5-benzyl-2-*tert*-butyl-3-methylimidazolidin-4-one (*MacMillan's* second generation catalyst), and *cis*/*trans*-5-benzyl-2-styryl-3-methylimidazolidin-4-one are reported. In the 2,2-dimethyl and in the *cis*-2-styryl derivative, respectively, a C-H bond of the *cis*-substituent in 2-position points to the center of the benzene ring of the benzyl group above the five-membered ring. NMR measurements provide evidence that the same structure/conformation is present in the solution. In the *cis*-2-(*tert*-butyl) derivative, the benzyl group is located over the iminium π-system. Overlays with DFT-calculated crotonylidene analogs show that the theoretical and experimental structures are almost superimposable. The structures are discussed in view of their role as reactive intermediates in organocatalysis and in view of the help synthetic organic chemists may experience from theory. Grošelj U.; Schweizer W. B.; Ebert M.-O.; Seebach D.; *Helv. Chim. Acta* 2009, *92*, 1–13) (*OK21*).

Several structures of the reactive intermediates (enamines and iminium ions) of organocatalysis with diarylprolinol methyl and silyl ethers (most of them are well established commercially available catalysts, *cf*. *Jørgensen's* 2-[bis(3,5-bistrifluoromethylphenyl)trimethyl-silanyloxym ethyl]pyrrolidine catalyst) have been determined. These reactive intermediates were synthesized/isolated and fully characterized. Iminium salts with $BF_4$, $PF_6$, $SbF_6$, and the weakly coordinating $Al[OC(CF_3)_3]_4$ anion were prepared. X-Ray crystal structures of enamine and of six iminium salts have been obtained and are described herein and in a previous preliminary communication (*Helv. Chim. Act*a 2008, *91*, 1999). According to the NMR spectra (in $CDCl_3$, ($D_6$)DMSO, ($D_6$)acetone, or $CD_3OD$), the major isomers of the iminium salts have (*E*)-configuration of the exocyclic N=C(1') bond, but there is up to 11% of the (*Z*)-isomer present in these solutions. In all crystal structures, the iminium ions have (*E*)-configuration, and the conformation around the exocyclic N-C-C-O bond is synclinal-*exo*, with one of the phenyl groups over the pyrrolidine ring, and the RO group over the π-system. One of the *meta*-substituents (Me or $CF_3$) on a 3,5-disubstituted phenyl group is also located in the space above the π-system. DFT calculations at various levels of theory confirm that the experimentally determined structures are by far the most stable ones (up to 8.3 kcal/mol). Implications of the results with respect to the mechanism of organocatalysis by diarylprolinol derivatives are discussed. (Grošelj U.; Seebach D.; Badine D. M.; Schweizer W. B.; Beck A. K.; Krossing I.; Klose P.; Hayashi Y.; Uchimaru T.; *Helv. Chim. Acta* 2009, *92*, 1225–1259) (*OK24*).

## 6. REVIEW ARTICLES

- STANOVNIK, Branko. Alkyl 3-(dimethylamino)propenoates and related enaminones in the synthesis of heterocyclic systems. V: EDER, Maria (Ed.). *20. Jahre Europäische Akademie der Wissenschaften und Künste : Festschrift*, (Edition Weimar, Book series of European Academy of Sciences and Arts, Vol. 13). Weimar: VDG, Verlag und Datenbank für Geisteswissenschaften, 2009, pp. 247–269. (*OK76*).
- WAGGER, Jernej, KRALJ, David, SVETE, Jurij, STANOVNIK, Branko. Ethyl isothiocyanatoacetate. V: PAQUETTE, Leo A. (Ed.). *Encyclopedia of reagents for organic synthesis*. 2nd ed. Chichester: J. Wiley and Sons, 2009, pp. 4966–4969. (*OK72*).
- SEEBACH, Dieter, BECK, Albert K., CAPONE, Stefania, DENIAU, Gildas, GROŠELJ, Uroš, ZASS, Engelbert. Enantioselective preparation of [beta][sup]2-amino acid derivatives for [beta]-peptide synthesis. *Synthesis (Stuttg.)*, 2009, no. 1, pp. 1–32. (*OK56*).

β-Amino acids with a single side chain in the α-position ($\beta^2$-amino acids or H-$\beta^2$hXaa(PG)-OH; *i.e*., homo-amino acids with proteinogenic side chains) have turned out to be important components in β-peptides. They contribute to unique secondary structures, they are required for mimicking the structure and the activity of β-turn-forming α-peptides, and can be used for protecting α-peptides against the attack by aminopeptidases. In contrast to $\beta^3$-homo-amino acids, the $\beta^2$-isomers cannot be obtained simply by enantiospecific homologation of (natural) α-amino acids, and need to be prepared by enantioselective reactions, or sequences or transformations, which are presented herein. The various preparative methods are ordered according to the bond at the stereogenic center, which is formed in the stereoselective step, with the four strategic bonds being the C(2)-C(3) backbone bond, the C(2)-side-chain bond, the C(2)-H bond, and the C(1)-C(2) bond between the carboxylate and the α-carbon. In the most frequently employed methods, a chiral auxiliary group is attached to the carboxyl C(1) atom or to nitrogen in the 3-position, but there are also various enantioselective catalytic processes, including hydrogenation of suitable acrylates. An alternative to stereoselective synthesis, namely resolution of racemic mixtures (e.g. by biocatalysis), is also discussed. A critical comparison of the various methods and strategies is presented. For the peptide chemist, a list is included with the Cbz-, Boc-, and Fmoc-protected $\beta^2$-amino acid building blocks, ready for peptide coupling. In addition, the search strategy for nonracemic $\beta^2$-amino acids and their precursors from the databases is described in detail.

- SVETE, Jurij. (4R*,5R*)-4-benzoylamino-5-phenyl-3-pyrazolidinone: a useful building block in the synthesis of functionalized pyrazoles. V: HORVAT, Monika A. (Ed.). *Stereochemistry research trends*. New York: Nova Science Publishers, cop. 2008, pp. 129–193, graphs (*OK75*).

A review on (4*R**,5*R**)-4-benzoylamino-5-phenyl-3-pyrazolidinone (**1**) as a useful and easily available building block for the synthesis of functionalized pyrazoles containing an *α*-amino acid or a dipeptide structural motif. The most useful derivatives of **1** are stable its azomethine imines **2**, obtained in the reactions of **1** with aromatic aldehydes. Within this context, [3+2] cycloadditions of azomethine imines **2** were the most extensively studied. Dipoles **2** exhibit broad reactivity (connectivity) spectrum, where most of their cycloaddition reactions are highly stereoselective. High selectivity of cycloadditions and simplicity of isolation of the products enable combinatorial solution-phase synthesis of pyrazolo[1,2–*a*]pyrazolone-type peptidomimetics with variable amino acid sequence and variable, yet predictable configuration.

## OTHER RELEVANT ACHIEVEMENTS

### A) EDITORIAL WORK

- PEJOVNIK, Stane, STANOVNIK, Branko (Ed.). *90 let kemijskih študijev na Univerzi v Ljubljani : 1919–2009*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2009. 159 pp., ilupp. ISBN 978-961-6756-10-5. (*OK89*).
- 13th Blue Danube Symposium on Heterocyclic Chemistry, Bled, September 20–23 2009, Slovenia, STANOVNIK, Branko (Ed.), SVETE, Jurij (Ed.). *Program. Abstracts of papers. List of participants*. Ljubljana: Organizing Committee, 2009. 163 pp., ilupp. (*OK90*).
- PANICO, Robert (Ed.), POWELL, Warren H. (Ed.), RICHER, Jean-Claude (Ed.), STANOVNIK, Branko (Ed.), TIŠLER, Miha (Ed.). *Vodnik po nomenklaturi organskih spojin IUPAC : priporočila 1993 (vključno s spremembami glede na nomenklaturo organske kemije IUPAC 1979)*. Ponatis izd. iz leta 1999. Ljubljana: Slovenska akademija znanosti in umetnosti, 2009. IX, 185 pp., ilupp. ISBN 978-961-6242-24-0. (*OK91*).
- *Acta chimica slovenica*. Svete, Jurij (guest editor 2009). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: = Slovenian Chemical Society, 1993–. ISSN 1318–0207. (*OK94*).

## B) PLENARY AND INVITED LECTURES

- STANOVNIK, Branko. [beta]-Dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related enaminones. Versatile reagents for preparation of various heterocyclic systems including natural products : [invited lecture]. V: *The 10th Annual Florida heterocyclic and synthetic conference : march 8th – march 11th, 2009*. [S. l.: s. n.], 2009, pp. 52. (*OK58*).
- WAGGER, Jernej, SVETE, Jurij, STANOVNIK, Branko. 3-Dimethylamino-2-acylamino and related enaminones in the synthesis of natural products : [invited lecture]. V: *9. Tagung Iminiumsalze, 7.–10. September 2009 in Bartholomä/Ostalbkreis, "Sport- und Bildungszentrum Bartholomä" : IMSAT-9*. [S. l.: s. n.], 2009, pp. 30–36. (*OK59*).
- SVETE, Jurij. Enaminones in combinatorial synthesis of heterocycles : [invited lecture]. V: *9. Tagung Iminiumsalze, 7.–10. September 2009 in Bartholomä/Ostalbkreis, "Sport- und Bildungszentrum Bartholomä" : IMSAT-9*. [S. l.: s. n.], 2009, pp. 6–15. (*OK62*).
- STANOVNIK, Branko. [beta]-Dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related enaminones : versatile reagents for preparation of various heterocyclic systems : [plenary lecture]. V: The Transmediterranean Colloquium on Heterocyclic Chemistry, 5–7 November 2009, Laico Hotel, Yasmine Hammamet. *Lectures and communications abstracts participants' list : TRAMECH 6*. [S. l.: s. n.], 2009, pp. Lecture 5. (*OK60*).
- WAGGER, Jernej, GOLIČ GRDADOLNIK, Simona, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. Enaminones in the synthesis of some unsaturated tryptophan ([triangle]Trp) containing alkaloid analogues : [invited Blue Danube lecture]. V: STANOVNIK, Branko (Ed.), SVETE, Jurij (Ed.). 13th Blue Danube Symposium on Heterocyclic Chemistry, Bled, September 20-23 2009, Slovenia. *Program. Abstracts of papers. List of participants*. Ljubljana: Organizing Committee, 2009, pp. 36. (*OK63*).

## C) LECTURE AT FOREIGN UNIVERSITIES OR RESEARCH INSTITUTIONS

STANOVNIK, Branko. *[beta]-Dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related enaminones – versatile reagents for preparation of various heterocyclic systems including natural products : [Bulgarian Academy of Sciences, Sofia, Bulgaria, 7th April, 2009]*. Sofia, 2009. (*OK82*).

## D) ORGANIZATION OF AN INTERNATIONAL SYMPOSIUM

In the year 2009 we organized an international symposium 13th Blue Danube Symposium on Heterocyclic Chemistry which has taken place at Bled from September 20 to September 23, 2009. Chairman of the International Scientific Committee B. Stanovnik, chairman of the Organizing Committee B. Stanovnik, vice-chairman J. Svete

## E) INTERNATIONAL RECOGNITION

B. Stanovnik:

2009 Medal awarded by the Tunisian Chemical Society, Hammamad, Tunisia

## F) MEMBERSHIP IN SCIENTIFIC COMMITTEES OF INTERNATIONAL CONFERENCES AND SYMPOSIA AND OTHER ADMINISTRATIVE FUNCTIONS

B. Stanovnik:

a) Chairman of the Advisory Editorial Board, Vestnik Slovenskega kemijskega društva, (since 1994 Acta Chimica Slovenica) Slovenia
b) Associate Editor, Bull. Soc. Chim. Belges, Belgium
c) Member of the Advisory Board, Croatica Chemica Acta, Croatia
d) Member of the Scientific Committee, European Colloquia on Heterocyclic Chemistry
e) Member of the Scientific Committee, Blue Danube Symposia on Heterocyclic Chemistry
f) Member of the Advisory Editorial Board, Journal of Heterocyclic Chemistry, USA
g) 1998–2004 Member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons, Den Haag, The Netherlands
h) Member of the Board of Electronic Journal ARKIVOC
i) Head, Department of International Relations and Scientific Coordination of the Slovenian Academy of Sciences and Arts
j) Member of the Advisory Board of the Advances in Heterocyclic Chemistry
k) Member of the Scientific Committee of TRAMECH Symposia (Transmediterranean Symposia of Heterocyclic Chemistry)
l) Member of the International Advisory Committee of Ibn Sina International Conferences On Pure and Applied Heterocyclic Chemistry, Egypt
m) Decanus Classis Scientiarum Naturalium Academiae Scientiarum et Artium Europeae, Salzburg. (Dean of the Class "Natural Sciences" of the European Academy of Sciences and Arts, Salzburg and Legatus EASA)
n) Member of the Scientific Committee of Eurasian Meetings on Heterocyclic Chemistry
o) Member of the Advisory Editorial Board, Trends in Heterocyclic Chemistry

# FIZIKALNA KEMIJA
## PHYSICAL CHEMISTRY

### PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

**P1–0201**

### VODJA PROGRAMSKE SKUPINE / PRINCIPAL RESEARCHER

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# POROČILO O REALIZACIJI PROGRAMA

## CILJI IN OSREDNJE TEME PROGRAMA

Tu navedene raziskave prispevajo k razumevanju fizikalno−kemijskih procesov, ki se dogajajo v živih bitjih in/ali so pomembni v industriji. Zanimajo nas raztopine in suspenzije nanodelcev, predvsem elektrolitov in polielektrolitov. Nekateri od slednjih so biološko pomembni (proteini in DNK), drugi, na primer, 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. V letu 2009 smo objavili 37 člankov, večino v znanstvenih revijah z visokim faktorjem vpliva.

## ZNANSTVENI DOSEŽKI

### 1. TEORETIČNE IN EKSPERIMENTALNE RAZISKAVE DISPERZNIH SISTEMOV

Z računalniško simulacijo Monte Carlo (MC) ter z integralskimi enačbami na osnovi replika Ornstein-Zernikove enačbe (ROZ) smo proučevali porazdelitev mešanice elektrolitov med nanoporoznim adsorbentom in nemoteno raztopino (preferenčna adsorpcija) (*FK36*). Izračunali smo fazni diagram za sistem, ki ga sestavljajo Lennard-Jonesove kroglice. Lastnosti trdne faze smo opisali s celično teorijo, parno in tekočo fazo pa s pomočjo termodinamične perturbacijske teorije (*FK7*).

Z metodo MC ter z Ornstein-Zernike-ovo integralsko enačbo smo, v kombinaciji z različnimi približki, proučevali strukturne lastnosti modelnih koloidnih disperzij s privlačnimi koloidnimi delci. Interakcije med koloidi smo modelirali z Baxterjevim modelom adhezivnih kroglic. Obravnavali smo urejanje privlačnih koloidnih delcev dvokomponentne koloidne disperzije ob togi trdni površini (*FK5*), ter določali prispevek enokomponentnega (*FK14*) in dvokomponentnega (*FK16*) adhezivnega topila k sili med koloidnimi delci. Sila v odvisnosti od razdalje med koloidnimi delci je kazala nihajoč odbojni in privlačni značaj s periodo enako velikosti molekul topila. Pri dovolj močnih privlačnih interakcijah med molekulami topila, postane sila daljnosežna in privlačna pri vseh razdaljah med koloidi. Rezultati so pomembni za razumevanje stabilnosti koloidnih disperzij. S primerjavo med rezultati teorije in simulacije smo ugotovili, da veljavnost teorije pojema z naraščajočo jakostjo privlačnih meddelčnih interakcij.

Raziskali smo modelni sistem, kjer se raztopina, ki vsebuje dvovalentne ione s prostorsko ločenim nabojem, nahaja med dvema ravnima nabitima površinama. Pri delu smo uporabili MC računalniško simulacijo ter posebej za obravnavo ionov s prostorsko ločenim nabojem prirejeno Poisson–Boltzmannovo enačbo. Ugotovili smo, da dvovalentni ioni lahko tvorijo »mostičke« med nabitima površinama in na ta način ustvarijo privlak med njima. Pri določeni razdalji med nabojema v divalentnih ionih smo opazili nastanek prenabitja na nabitih površinah, kar je lahko eden izmed mehanizmov za nastanek privlaka, med sicer enako nabitimi koloidnimi delci (*FK30*).

## 2. RAZTOPINE ELEKTROLITOV IN POLIELEKTROLITOV

S pomočjo študija dinamike molekul smo izračunali potencial povprečne sile med ioni prve in sedme skupine periodnega sistema v vodi (*FK27, FK37*). Uporabili smo štiri različne modele vode in več modelov ionov (glej sliko na naslovnici št. 19 vol. 113) (*FK27*). Izračunali smo konstante asociacije za posamezne pare in rezultate primerjali z rezultati dobljenimi s pomočjo meritev prevodnosti. Na ta način smo želeli preveriti veljavnost posameznih modelov vode in ionov.

V članku (*FK25*) smo raziskovali dinamiko ionov in molekul v raztopinah tetraalkilamonijevih soli. Pokazali smo, da na lastnosti teh soli, ki so izrazito odvisne od vrste aniona, vplivajo tako hidrofobne kot tudi ionske skupine.

Dodatek raztopine polielektrolita močno vpliva pogostost trkov med istoimenskimi ioni. V članku (*FK2*) smo proučili raztopino z dvovalentnimi protiioni. Poliion smo opisali kot enakomerno nabit valj, ione kot nabite kroglice, vodo pa kot zvezno snov z dielektrično konstanto čiste vode.

Z metodo dielektrične relaksacijske spektroskopije (DRS) smo raziskali interakcije med kationskimi polielektroliti (ioneni) in protiioni v vodnih raztopinah v odvisnosti od gostote naboja poliiona in vrste protiiona (*FK33, FK34*).

S konduktometričnimi, potenciometričnimi, kalorimetričnimi in fluorescenčnimi meritvami smo študirali vedenje vodnih raztopin polietakrilne kilsine, PEA, pri 25 ºC (*FK23*). Rezultati so pokazali, da so kratke verige PEA v vodi močno asociirane v vsem območju stopnje ionizacije karboksilnih skupin, kar smo pripisali tvorbi vodikovih vezi med neioniziranimi skupinami in prisotnosti hidrofobnih etilnih skupin na verigi.

Transportne lastnosti polianetolesulfonske kisline in njenih soli smo proučili v članku (*FK24*). Pokazali smo, da se polianetolisulfonati vedejo podobno kot soli polistirenske kisline. Nekoliko manjše vezanje protionov v primerjavi s polistirensulfonati je moč pripisati manjši gostoti naboja na polianetolesulfonatnem anionu.

V sodelovanju z raziskovalci s Karlove univerze v Pragi (Češka republika) smo raziskovali optične in transportne lastnosti vodnih raztopin poli(3-tiofen ocetne kisline) *(FK39*). Izmerili smo električno prevodnost polielektrolita in transportna števila makroiona pri 25 ºC ter iz teh podatkov izračunali delež prostih ionov. Analiza absorpcije v vidnem delu svetlobnega spektra je potrdila, da se omenjeni polielektrolit s konjugiranimi dvojnimi vezmi vede podobno kot ostali polielektroliti.

## 3. POVRŠINSKO AKTIVNE SNOVI (PAS)

V preglednem članku (*FK40*) smo povzeli rezultate povezane s strukturo čistih enostavnih alkoholov, strukturo binarnih sistemov alkohol/voda in vplivom alkoholov na strukturo sorodnih ternarnih sistemov z neionskim surfaktantom. S pomočjo rezultatov simulacije MC smo računali rentgensko sipanje za modelne primarne aldehide od propanala do nonanala ter izračunane vrednosti primerjali z eksperimentalnimi rezultati (*FK28*). Ti rezultati so osvetlili povezavo med mikroskopsko in mezoskopsko strukturo molekularnih raztopin. Izvedena je bila tudi kombinirana eksperimentalno-teoretična raziskava strukture in specifičnih interakcij parov surfaktant-polielektrolit v vodnih raztopinah neionskega surfaktanta in anionskega konjugiranega polielektrolita (*FK31*). Raziskali smo tudi vplive različnih soli na vodne raztopine človeškega serumskega albumina (*FK8*) in strukturo mešanih micelov neionskega surfaktanta C12E5 in troblok-kopolimera P123 (*FK26*).

Preučevali smo hierarhično organizirane sisteme v obliki notranje samo-organiziranih emulzij (ISAmulzij; angl. 'internally self-assembled emulsions') oziroma termo-reverzibilnih ISAmulzija-gelov (*FK18, FK32*), ki so potencialno uporabni v farmacevtski in prehrambeni industriji.

Izvedli smo termodinamsko raziskavo vpliva temperature in dodane soli (NaCl) na micelizacijo kationskega surfaktanta dodeciltrimetilamonijevega klorida (DTAC) v vodi (*FK19*). Ugotovili smo, da kritična micelna koncentracija pada z naraščajočo koncentracijo NaCl, kar lahko pripišemo senčenju elektrostatskega odboja med nabitimi deli molekule surfaktanta. Proces je endotermen pri nizkih in eksotermen pri visokih temperaturah, kar je posledica razmerja entalpijskega in entropijskega prispevka zaradi hidrofobnega efekta.

Proučevali smo strukturo farmacevtsko uporabnih »čistih« mikroemulzij ter mikroemulzij z vgrajenim celekoksibom (*FK3*) ter ibuprofenom (*FK41*). Merili smo tudi hitrost in obseg sproščanja učinkovin iz posameznih mikroemulzijskih struktur ter ugotovili, da je sproščanje odvisno tako od mikrostrukture kot od solubilizacijske kapacitete sistema in ga je v določeni meri mogoče napovedati.

## 4. HIDRATACIJA PREPROSTIH IN SESTAVLJENIH TOPLJENCEV

S pomočjo preprostega dvodimenzionalnega modela vode (MB) smo študirali vpliv soli na topnost hidrofobnega topljenca v odvisnosti od njegove velikosti (*FK10*). Z MB modelom vode v treh dimenzijah smo z metodo Monte Carlo, Wertheimovo integralsko enačbo in termodinamično perturbacijsko teorijo izračunali lastnosti čiste vode. Teoriji se pri višjih temperaturah dobro ujameta s simulacijami (*FK17*).

Z metodo simulacije dinamike molekul smo v dveh člankih (*FK15, FK29*) raziskovali hidratacijo hidrofobnih polielektrolitov (3,3 in 6,6 ionenov) v prisotnosti različnih soli. Pokazali smo, da hidrofobne skupine prispevajo k znižanju osmoznega koeficienta in tako pojasnili slabo ujemanje klasičnih teorij s poskusi.

## 5. KVANTNA KEMIJA IN MOLEKULSKA PODOBNOST

Z uporabo računalniških simulacij molekulske dinamike smo opravili i) termodinamske in strukturne raziskave vezave netropsina na sedem različnih baznih zaporedij v ožjem kanalu DNA. Rezultati so pokazali, da razlik v jakosti vezave netropsina na dana bazna zaporedja ni mogoče razložiti samo z vidika vodikovih vezi in interakcijskih energij med ligandom in DNA, temveč je pri razlagi potrebno upoštevati tudi spremembe v solvataciji ter entropijske spremembe, do katerih pride pri tvorbi kompleksov ligand-DNA. ii) izboljšavo modelne strukture peptida GCN4p16-31, za katero smo ugotovili, da zbirka struktur, ki so dostopne v proteinski banki PDB ne zadovoljuje vseh meritev NMR, t.j. NOE razdalj med vodikovimi atomi v molekuli GCN4p16-31 ter $^3$J-sklopitvenih konstant. Pokazali smo, da se konfiguracije obravnavanega peptida ujemajo z meritavmi NMR le, če se pri izračunu strukture upošteva časovno povprečenje NOE razdalj in $^3$J-sklopitvenih konstant. Analiza izračunanih struktur je pokazala, da je konfiguracijski prostor molekule GCN4p16-31 mnogo večji od konfiguracijskega prostora, ki ga predstavljajo strukture objavljene v proteinski banki PDB. Članka, vezana na te raziskave, sta v recenziji.

V okviru projekta FIRB RETI RBPR05NWWC_04 je dr. Podlipnik od 1. junija do 31. oktobra 2009 gostoval v skupini profesorja P. Senecija na inštitutu CISI, ki deluje v okviru Milanske univerze. Raziskave, opravljene v tem obdobju, bodo koristile pri razvoju novih kinaznih inhibitorjev.

Na tem področju je pomembno tudi delo: »Hidrotrioksidi namesto cikličnih tetraoksidov (tetraoksolanov) kot začetni reakcijski intermediati pri nizkotemperaturni ozonaciji aldehidov« (*FK22*).

## 6. RAZISKAVE BIOLOŠKO POMEMBNIH MOLEKUL

Prispevali smo k molekularni razlagi in razumevanju pojavov v zvezi z delovanjem bakterijskih modulov toksin-antitoksin, pomembnih za življenje in smrt bakterijskih celic. Uspeli smo neposredno povezati termodinamiko zvitja/razvitja toksina CcdB, ki povzroča celično smrt bakterij, z njegovimi strukturnimi značilnostmi (*FK4*). S pomočjo študija termodinamike vezanja in odgovarjajočih strukturnih informacij smo opredelili gonilne sile prepoznavanja giraze s toksinom CcdB (*FK12*). Raziskali smo termodinamiko in mehanizem zvitja/razvitja proteina MazG, regulatorja delovanja modula toksin–antitoksin, ki vpliva na preživetje bakterijskih celic pod stresnimi pogoji (*FK21*).

Ekskluzivno praktično in teoretično znanje s področja spektroskopije in kalorimetrije s pridom uporabljamo pri reševanju industrijske problematike, v katero smo vključeni preko sodelovanja s farmacevtsko firmo Lek (BIO – 05/2007 in BIO – 05/2009).

## 7. FARMACEVTSKO POMEMBNI TOPLJENCI

Proučevali smo transportne lastnosti vodnih raztopin učinkovin salicilat, ibuprofen, diklofenak in naproksen natrijeve soli ter diklofenak kalijeve soli (*FK1*) ter nekaterih tetra-n-alkilamonijevih cikloheksilsulfamatov (*FK9*). Razliko v mobilnosti preiskovanih ionov smo pripisali različni hidrataciji ter možnim hidrofobnim interakcijam.

### 8. IONSKE TEKOČINE

Raziskovali smo asociacijo ionov v razredčenih raztopinah ionskih tekočin 1-butil-3-metilimidazolijevega klorida in tetraflouroborata v metanolu in DMSO. Obe ionski tekočini kažeta zmerno asociacijo v metanolu in bistveno šibkejšo v DMSO (*FK13*).

## DRUGI RELEVANTNI DOSEŽKI

1. Imeli smo več uvodnih predavanj na mednarodnih konferencah doma (Vlachy, V: »Kako velikost ionov in prisotnost nepolarnih skupin vplivata na lastnosti raztopin elektrolitov v vodi«, SKD, Maribor 2009) in tujini (Vlachy, V. »Ionenes, hydrophobic polyelectrolytes with unusual solution thermodynamic properties«; 31. ICSC : Innsbruck, 2009). O svojem delu smo poročali na tujih univerzah in inštitutih kot so UC San Francisco, Vrije Universiteit Amsterdam, University of Helsinki, University of Regensburg, University Pierre and Marie Curie Paris, ETH Zürich, in še na nekaterih drugih ustanovah doma in v tujini.
2. M. Bešter Rogač je sourednica in občasno (2009, vol. 56/1) tudi gostujoča urednica revije Acta Chimica Slovenica (*FK57*).
3. Dva člana PS sta bila v tem obdobju na študijskem izpopolnjevanju v tujini (Jožica Dolenc – ETH Zürich, Črtomir Podlipnik – CISI, Milano).
4. Sodelovali smo v bilateralnih projektih z Avstrijo, Madžarsko, Hrvaško, Portugalsko, ZDA, in Francijo.
5. Kot partnerji univerze v San Franciscu sodelujemo pri projektu »Solvation in Biology«, ki ga že deveto leto zapored financira National Institute of Health, ZDA.
6. Sodelovali smo tudi pri treh COST projektih (D31 G. Vesnaver, D43 M. Bešter Rogač in MP0802 J. Lah).

## RESEARCH PROGRAMME REPORT

### PROGRAMME GOALS

The results of this research contribute toward better understanding of physico-chemical processes in living beings or/and technologically important processes. Our research focus is on nanoparticles in solutions. 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 to our colleagues in industry. During the last year we published 37 scientific papers, mainly in distinguished journals with high impact factor.

# RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

## 1. THEORETICAL AND EXPERIMENTAL STUDIES OF DISPERSED SYSTEMS

Monte Carlo (MC) simulation, and integral equation theories based on the “replica” Ornstein-Zernike equation (ROZ) have been used to study the distribution of electrolyte mixtures between bulk solutions and charged nanoporous adsorbent (preferential adsorption) (*FK36*). Phase diagram of Lennard-Jones spheres was constructed. The solid phase was described by the cell theory, while the liquid and gas phase properties were calculated using the thermodynamic perturbation theory (*FK7*).

Monte Carlo (MC) simulation and Ornstein–Zernike integral equation theory supplemented by various closures were used to study structural properties of model colloidal dispersions comprising attractive colloidal particles. Inter–particle interactions were modeled by Baxter’s adhesive hard sphere model. Ordering of attractive colloidal particles of a two-component colloidal dispersion near a planar hard plate was studied (*FK5*) and the contributions of one–component (*FK14*) and two-component (*FK16*) solvents to the force between the colloids were explored. The effective force between the colloidal particles showed oscillatory repulsive and attractive character, with the period equal to the molecular diameter of the solvent molecules. At sufficient strength of the inter-particle stickiness, these oscillations disappeared, the force becoming long–ranged and attractive at all separations. The results yield better understanding of the stability of colloidal dispersions. The agreement between the theoretical predictions and simulation data was found from fair to very good, and decreased by increasing the strength of attractive inter–particle interactions.

In this theoretical study a model solution containing short divalent ions with spatially separated charges was placed in a gap between two equally charged plates which mimic a surface of charged colloidal particles. The Poisson-Boltzmann equation, modified to study rigid divalent ions, was used to study the model along with the canonical MC computer simulations. The results show that orientation ordering of rigid (rodlike) divalent counterions provides an effective attraction between the two charged plates. At a certain length of divalent ions, an overcharging of plates was observed. The effect is identified as a possible mechanism of an effective attraction between the charged colloidal particles (*FK30*).

## 2. ELECTROLYTES AND POLYELECTROLYTES

MD simulation is used to calculate the potential of mean force for alkali halides in explicit water (*FK27, FK37*). Four different models of water and several different force fields to describe ions were used (see also the front page of JPC B no. 19, vol. 113) (*FK27*). The association constants were calculated for different combinations of cations and anions. The results were compared with the association constant determined from the conductivity measurements to establish the validity of different force fields.

In the paper (*FK25*) we described the dynamics of ions and water molecules in solutions of tetraalkylammonium salts. The solution properties of these salts are highly anion-specific, depending on the number of hydrophobic groups present.

Addition of polyelectrolyte to simple electrolyte solution strongly modifies the collision frequency between equally charged ions. In this contribution (*FK2*) we studied a model solution with polyions pictured as infinitely long and uniformly charged cylinders, while the ions were charged as hard spheres, and water as a continuum with a dielectric constant of pure water.

Dielectric relaxation spektroscopy (DRS) was used to study the interaction between cationic polyelectrolytes (x,y ionenes) and various counterions as a function of the charge density of ionenes (*FK33, FK34*).

The behavior of poly(α-ethyl acrylic acid), PEA, was studied in aqueous solutions at 25 ºC by conductometric, potentiometric, calorimetric, and fluorescence measurements (*FK23*). The results show that short PEA chains are strongly associated in water in the whole range of degrees of ionization of carboxyl groups. Intermolecular association was ascribed to the formation of hydrogen bonds between unionized groups with a favorable contribution of the hydrophobic ethyl side–groups.

Transport properties of polyanetholesulfonic acid (HPAS) and its salts in water were studied in (*FK24*). The behavior of these solutions resembles that of polystyrenesulphononates. A somewhat smaller binding of counterions in HPAS and its salts can be attributed to a smaller charge density (larger radius) of this polyanion.

In collaboration with the research group from Charles University, Prague (Czech Republic) we investigated optical and transport properties of aqueous solutions of poly(3-thiophene acetic acid) (*FK39*). In this study the electric conductivity of the solution and transport numbers of the macroion were measured at 25 ºC. On the basis of these data the degree of free counterions was calculated. The analysis of absorption spectra in the visible region confirmed that this polyelectrolyte has similar features as other polyelectrolytes.

## 3. SURFACTANT STUDIES

In the review (*FK40*) the results on the structure of pure simple alcohols, structure of binary water/alcohol mixtures and various effects of the simple alcohols on the related ternary systems of nonionic surfactant were summarized. Using the configurational-bias MC simulations of the model aldehydes (transferable potential for phase equilibria-united atom model) and experimental small–angle x–ray scattering (SAXS) method we investigated the structure of the primary liquid aldehydes from propanal to nonanal (*FK28*). With these results we could better understand the connection between the microscopic and mesoscopic structure of these molecular solutions. A combined experimental and theoretical investigation of the structure and specific surfactant-polyelectrolyte interactions in aqueous solutions of nonionic surfactant and anionic conjugated polyelectrolyte was also conducted (*FK31*). Similarly, the salt-specific effects of various simple inorganic salts on human serum albumin in aqueous solutions (*FK8*) and the structure of mixed nonionic surfactant C12E5/triblockcopolymer P123 micelles (*FK26*) were investigated.

We have studied the hierarchically structured, internally self-assembled emulsions (ISAmulsions) and successfully promoted their hierarchical structure for one level in a sense of thermo–reversible ISAmulsion–hydrogels (*FK18, FK32*), which are potentially applicable in pharmaceutical and food industry.

Thermodynamics of micelle formation of the cationic surfactant dodecyltrimethylammonium chloride (DTAC) in water and aqueous NaCl solutions at different temperatures was investigated (*FK19*). It was found out that the critical micelle concentration decreases by increasing the concentration of NaCl, indicating a progressive screening by Cl ions of the electrostatic repulsion between ionic head groups of the surfactant. The enthalpy of micellization passes through zero in all the systems investigated at approximately the same temperature at which the cmc reaches a minimum. This can be ascribed to the balance between the enthalpy and entropy in the micellization process, arising mainly from the hydrophobic effect.

Structural transformations were investigated in unloaded and celecoxib- (*FK3*) and ibuprofen-loaded (*FK41*) pharmaceutically applicable microemulsions. It was shown that the drug release from the microemulsions is influenced by the microstructure and solubilization capacity of the system, and can be predicted to a certain extent.

## 4. HYDRATION OF SIMPLE AND COMPLEX SOLUTES

A simple 2D water model (MB) was used to explain the influence of simple salts on the solubility of hydrophobes in water, depending on its size (*FK10*). The MB model in three dimensions was used to calculate the properties of bulk water via the Monte Carlo method, integral equations, and thermodynamic perturbation theory. The two theories are in good agreement with the simulation at high temperatures (*FK17*).

MD simulation approach was used (*FK15, FK29*) to study hydration of hydrophobic polyelectrolytes (3,3 and 6,6 ionenes) in the presence of various salts. We showed that the presence of hydrophobic groups lowers the osmotic coefficient of the solution and in this way explained a somewhat poor agreement between classical electrostatic theories and experimental data.

## 5. QUANTUM CHEMISTRY AND MOLECULAR SIMILARITY STUDIES

Using molecular dynamics simulations we performed: i) a parallel thermodynamic and structural study on netropsin binding to an AT- and to a set of 6 mixed AT/GC-containing binding sequences in the DNA minor groove. The results of the analyses reveal that the sequence–specific netropsin-DNA binding affinities cannot be explained solely in terms of ligand–DNA hydrogen bonding or interaction energies. Changes in solvation and entropy upon binding also show sequence-specific contributions to the free energy of binding and provide a more complete picture of various factors which determine binding; ii) structure refinement of a peptide GCN4p16-31 for which we have shown that the proposed set of 20 NMR model structures does not reproduce all the measured NOE upper distance bounds and $^3$J-coupling constants. We found out that only configuration ensembles, obtained by applying simultaneously time-averaged NOE distance and $^3$J-coupling constant restraining, reproduce all the experimental data. The analyses of the simulated ensembles show that the conformational variability of GCN4p16-31 in a solution admitted by the available set of NMR data is larger than represented by the set of NMR model structures which is currently deposited in the Protein Data Bank. Two manuscripts summarizing these studies were submitted for publication.

Dr. Podlipnik acted as visiting professor at the Prof. P. Seneci group (CISI, University of Milano) from June, 1st to October 31st 2009. Within the framework of the FIRB RETI RBPR05NWWC_04 project they examined the possibilities of developing new kinase inhibitors.

We studied hydrotrioxides rather than cyclic tetraoxides (tetraoxolanes) as the primary reaction intermediates in the low-temperature ozonation of aldehydes (*FK22*).

### 6. BIOLOGICALLY IMPORTANT MOLECULES

We have contributed to molecular interpretation and understanding of a phenomena related to the functioning of toxin-antitoxin modules that are important for bacterial life and death. We directly correlated thermodynamics of folding/unfolding of the toxin CcdB which causes cell death, to its structural features (*FK4*). We estimated the driving forces of gyrase recognition by the toxin CcdB on the basis of thermodynamic binding studies and the corresponding structural information (*FK12*). We investigated the thermodynamics and the mechanism of folding/unfolding of protein MazG a regulator of one toxin–antitoxin module that influences the bacterial cell survival under stress conditions (*FK21*).

Exclusive practical and theoretical knowledge in spectroscopy and calorimetry has been successfully used in solving industrial problems through well established collaboration with the pharmaceutical company Lek (BIO – 05/2007 in BIO – 05/2009).

### 7. PHARMACEUTICALLY IMPORTANT SOLUTES

Transport properties of anti-inflammatory drugs salicylate, naproxen, ibuprofen sodium and diclofenac sodium salts and diclofenac potassium salt (*FK1*) and of some tetraalkyl ammonium cyclohexylsulfamates (*FK9*) were studied in aqueous solution. The results are discussed in terms of hydration properties of the solutes and possible hydrophobic interaction.

### 8. IONIC LIQUIDS

Ion association of dilute solutions of the ionic liquids (IL) 1-butyl-3-methylimidazolium chloride and 1-butyl-3-methylimidazolium tetrafluoroborate in methanol and DMSO were studied (*FK13*). The ILs examined here exhibit moderate association in methanol, and weak association in DMSO.

## OTHER RELEVANT ACHIEVEMENTS

1. During the last year we delivered two keynote lectures at domestic and international scientific conferences (Vlachy, V: “Kako velikost ionov in prisotnost nepolarnih skupin vplivata na lastnosti raztopin elektrolitov v vodi”, SKD, Maribor 2009; Vlachy, V. “Ionenes, hydrophobic polyelectrolytes with unusual solution thermodynamic properties”; 31. ICSC: Innsbruck, 2009). We have delivered lectures at several foreign universities: UC San Francisco, Vrije Universiteit Amsterdam, University of Helsinki, University of Regensburg, University Pierre and Marie Curie Paris, ETH Zürich, and other institutions.
2. M. Bešter Rogač is a co-editor and occasionally a guest editor of the journal Acta Chimica Slovenica (*FK57)*.
3. Last year two members of the group were on longer study visits to foreign universities (Jožica Dolenc – ETH Zürich, Črtomir Podlipnik – University of Milano).
4. Through bilateral projects we maintain contacts with different research groups in Austria, Hungary, Croatia, Portugal, USA, and France.
5. For the last nine last years we have been partners in the project “Solvation in Biology” UC San Francisco, sponsored by the National Institute of Health.
6. We participated in three COST projects (D31 G. Vesnaver, D43 M. Bešter Rogač and MP0802 J. Lah).

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

### PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

**P1–0230**

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# POROČILO O REALIZACIJI PROGRAMA

## CILJI PROGRAMA

Cilj raziskovalnega programa je razvijanje sinteze spojin za znanstvene in aplikativne namene pod okolju čim bolj prijaznimi pogoji (zelena kemija) in z visoko atomsko ekonomičnostjo.

Program se tesno povezuje z več mednarodnimi programi, ki vključujejo raziskovalne skupine iz EU in ZDA, kot tudi z raziskovalnimi programi več domačih akademskih institucij (UL Medicinska fakulteta, UL Fakulteta za farmacijo, Kemijski inštitut) in industrijskih raziskovalnih ustanov (Krka, Lek). V letu 2009 je bilo naše raziskovalno delo usmerjeno v načrtovanje novih sinteznih metod, reagentov in reakcij, ki bi omogočile sintezo spojin s ciljnimi biološkimi aktivnostmi. Doc. dr. B. Štefane je v letu 2009 začel svoje krajše post-doktorsko izpopolnjevanje v ZDA.

## OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

Na področju cikličnih aminokislinskih derivatov smo raziskali dvojno Diels−Alderjevo cikloadicijsko reakcijo 2*H*-piran-2-onov z *N*-substituiranimi maleimidi ali z anhidridom maleinske kisline, ki daje biciklo[2.2.2]oktenske derivate. Pri tem smo opazili nenavaden vpliv velikosti obroča, pripojenega k 2*H*-piran-2-onom, na *ekso/endo* selektivnost te cikloadicijske reakcije. S primerno izbiro izhodnih spojin in reakcijskih pogojev (reakcije s konvencionalnim segrevanjem v refluktirajočem toluenu, dekalinu ali tetralinu in reakcije pod vplivom mikrovalov v topilih ali kot reakcije brez topil) lahko pripravimo *ekso*,*ekso* ali *ekso*,*endo* spojine kot edine produkte (*OK34*. K. Kranjc, F. Perdih, M. Kočevar, *J. Org. Chem.* 2009, *74*, 6303). Na osnovi naših rezultatov s tega področja smo pripravili pregledni članek, v katerem smo opisali obročne pretvorbe 2*H*-piran-2-onov in pripojenih piran-2-onov z nukleofilnimi reagenti (*OK55.* F. Požgan, M. Kočevar, *Heterocycles* 2009, *77*, 657). Opisali smo tudi novo hitro pretvorbo 5-acil-2*H*-piran-2-onov z različnimi amidini kot 1,3-binukleofili v izomerno čiste (*E*)-α,β-didehidro-α-aminokislinske (DDAA) derivate, ki so na β-položaju vsebovali 5-pirimidilno enoto. Postopek se izvaja v etanolni raztopini (ali v zmesi etanol/voda) in v prisotnosti $Na_2CO_3$ kot netoksične baze ter pod pogoji mikrovalovnega obsevanja. Če se izhaja iz 5-etoksikarbonil-2*H*-piran-2-onskih derivatov v prisotnosti DBU kot baze, nastanejo ustrezni pirano[2,3-*d*]pirimidini. Ta pretvorba predstavlja novost na področju sinteze doslej neznanih tipov nenasičenih aminokislinskih derivatov kot potencialnih intermediatov za pripravo novih tipov aminokislin (*OK49.* J. Hren, F. Požgan, A. Bunič, V. I. Parvulescu, S. Polanc, M. Kočevar, *Tetrahedron* 2009, *65*, 8216). Tako pripravljene spojine smo uporabili kot substrate za razvijanje novih metod kemoselektivnega katalitskega hidrogeniranja C=C dvojnih vezi. Kataliza, ki temelji na nanodelcih, je hitro razvijajoče se raziskovalno področje; njegov najpomembnejši del so trenutno metode zelene kemije. Pred kratkim so se pojavile metode, ki temeljijo na kombinaciji superkritičnega ogljikovega dioksida in ionskih tekočin kot reakcijskega medija. V članku smo objavili metodo za pripravo in zajetje rodijevih nanodelcev v enostavnih amonijevih soleh, ki sicer ne predstavljajo ionskih tekočin, vendar se, zaradi znižanja tališča, v prisotnosti $CO_2$ pretvorijo v ionske tekočine. Metoda izhaja iz kvaternih amonijevih halidov ali drugih soli ($R_4N^+X^-$), rodijevih spojin ([$Rh(acac)(CO)_2$], $RhCl_3$), vodika in ogljikovega dioksida, ki jih zmešamo v jeklenem reaktorju za visoke tlake. Tako se v matrici tvorijo nanodelci z definiranimi velikostmi delcev, ki so homogeno razporejeni v klastrih z velikostjo 1−4 nm; le-te smo uporabili kot selektivne katalizatorje za hidrogeniranje enostavnih substratov (cikloheksena in benzena) pa tudi za bolj aktualne DDAA derivate, ki se jih pod standardnimi pogoji ne da enostavno hidrogenirati. Nov katalitski sistem kaže do naših DDAA derivatov znatno drugačno obnašanje in selektivnost (C=C dvojna vez nasproti fenilni skupini) kot standardni homogeni ali heterogeni katalizatorji. Novi katalizatorji se dajo tudi enostavno ločiti iz reakcijske zmesi in reciklirati (*OK7.* V. Cimpeanu, M. Kočevar, V. I. Parvulescu, W. Leitner, *Angew. Chem. Int. Ed.* 2009, *48*, 1085). Te raziskave so nadaljevanje naših sistematičnih študij v okviru projektne skupine COST D24 »Synthesis and Application of New Ligands for Asymmetric Heterogeneous Catalysis (D24/0007/02)«. Tukaj smo pritegnili še partnerja iz Nemčije (prof. Walterja Leitnerja). Pomembno je še omeniti, da je prof. Leitner dobil za opisane rezultate od Nemškega kemijskega društva Wöhlerjevo nagrado za izjemne dosežke v kemiji v letu 2009 »za procese, ki ohranjajo naravne vire« (gl.: *Angew. Chem. Int. Ed.*, 2009, *48*, 6587).

Raziskali smo tudi reaktivnost $BF_2$-kompleksov 1,3-dikarbonilnih spojin pod reduktivnimi reakcijskimi pogoji. Metoda omogoča enostaven dostop do vrste 3-aril in heteroarilaldehidov in ketonov (*OK45.* B. Štefane, S. Polanc, *Tetrahedron* 2009, *65*, 2339). V sodelovanju s Fakulteto za farmacijo smo sintetizirali serijo spojin, ki kažejo inhibitorno aktivnost na AKR1C1 in AKR1C3 encime (*OK14.* B. Štefane, P. Brožič, M. Vehovc, T. Lanišnik-Rižner, S. Gobec, *Eur. J. Med. Chem.* 2009, *44*, 2563) V okviru sodelovanja smo prav tako uspeli najti spojino vodnico heterociklične strukture, ki se odlikuje z aktivnostjo na Mur F encim, ki igra pomembno vlogo v sintezi bakterijske celične stene (*OK27.* I. Sosič, B. Štefane, A. Kovač, S. Turk, D. Blanot, S. Gobec, *Heterocycles* 2010, *81*, 91).

Učinkovita metoda za sintezo pirazol-3-onov vključuje intramolekularno aminiranje ustreznih diazenov (*OK50.* B. Burja, M. Kočevar, S. Polanc, *Tetrahedron* 2009, *65*, 8690). Ta način je splošen za pripravo pirazol-3-onov iz lahko dostopnih propenojskih kislin. Slednje dobimo s Perkinovo reakcijo arilocetnih kislin z aromatskimi aldehidi in jih nato pretvorimo v odgovarjajoče hidrazide. Oksidacija le-teh daje diazene, ki pri obdelavi z $ZrCl_4$ ciklizirajo. Metoksikarbonilno zaščito dušika 1 v pirazolonskih derivatih odstranimo pod blagimi reakcijskimi pogoji. Opisana metodologija deluje enako uspešno s 3-substituiranimi in 2,3-disubstituiranimi propenojskimi kislinami, kar utegne odpreti nove poti do številnih derivatov biološko aktivnih spojin s prikondenziranim pirazolskim obročem.

Naša nedavna odkritja s področja diazenov in druge sorodne raziskave so opisane v prispevku, objavljenem v reviji *Synlett* (*OK42.* J. Košmrlj, M. Kočevar, S. Polanc, *Synlett* 2009, 2217). Diazeni so namreč enostavno dostopni dušikovi elektrofili, ki lahko služijo kot primerni reagenti za tvorbo dušik vsebujočih spojin. Članek je osredotočen na štiri vrste diazenov: dialkil diazendikarboksilate (včasih so jih imenovali dialkil azodikarboksilati), alkil ali arilaminokarbonildiazenkarboksilate, diazendikarboksamide (imenujejo jih tudi azodikarboksamidi) in diazenkarboksamide (znani so tudi kot azokarboksamidi). Publikacija opisuje razne vrste pretvorb z izjemo Diels-Alderjeve in Mitsunobujeve reakcije. Namen prispevka je prikazati uporabnost in mnogovrstnost diazenov v sintezne namene. Te spojine so namreč primerni gradniki, ki omogočajo enostavno in selektivno uvedbo dušikove funkcionalne skupine v različne organske molekule. Opisane so tudi elektrokemijske lastnosti in biokemijski aspekti diazenov.

V sodelovanju s Fakulteto za farmacijo UL, Univerzo v Warwicku in Univerzo v Leedsu smo načrtovali in sintetizirali nove majhne molekule – inhibitorje VanA in DdlB, ki imajo $IC_{50}$ vrednosti v mikromolarnem območju. Rezultati kažejo, da je fosfat na hidroksilni skupini hidroksietilaminskega izostera bistven za inhibicijo tako VanA, kot tudi DdlB. Načrtovane spojine predstavljajo pomembno izhodišče za nadaljnjo optimizacijo in modifikacijo, da bi izboljšali inhibitorne lastnosti proti VanA in DdlB. Te vrste inhibitorjev dajejo možnost za razvoj zdravil, ki bi jih uporabili v primerih bakterijske resistence na vancomicin. Nadalje, delovanje teh spojin proti VanA in DdlB nakazuje, da bo mogoče razviti učinkovine širokega spektra, ki bi bile uporabne tako za Gram-pozitivne, kot tudi za Gram-negativne infekcije (*OK10.* M. Sova, G. Čadež, S. Turk, V. Majce, S. Polanc, S. Batson, A. Lloyd, D. I. Roper, C. W. Fishwick, S. Gobec, *Bioorg. Med. Chem. Lett.* 2009, *19*, 1376).

V sodelovanju s farmacevtsko tovarno Lek d.d. smo razvili sintezo 3-acetamido-β-resorcilnih kislin kot potencialnih analogov platensimicina in kot inhibitorje FabF in FabH. Platensimicin je antibiotik izoliran iz *Streptomyces platensis*, ki deluje na bakterijske FabF encime, kateri nastopajo v biosintezi maščobnih kislin. Naša metoda je sestavljena iz enostavne dvostopenjske strategije, pri kateri se izognemo uporabi zaščitnih skupin. Izhaja iz 2-aminoresorcinola, ki se ga najprej *N*-acilira in potem karboksilira z uporabo modificirane metode Kolbe–Schmitt, uporabljajoč DMSO kot topilo in $K_2CO_3$ kot bazo, pri čemer nastanejo želene 3-acetamido-β-resorcilne kisline. Ta sintezna strategija omogoča pripravo knjižnice spojin potencialnih inhibitorjev FabF in FabH (*OK39.* N. Maraš, P. Štefanič Anderluh, U. Urleb, M. Kočevar, *Synlett* 2009, 437). Razvili smo tudi prvo sintezo (4*R*,6*S*)-4-(*terc*-butildimetilsililoksi)-6-formiltetrahidro-2*H*-piran-2-ona (aldehid **1**) in pokazali njegovo vrednost v sintezi statinov preko laktonske stranske verige. Aldehid **1** smo pripravili v njegovi hidrirani obliki (kot hidrat ali »carbonyl water adduct«), kar je omogočilo njegovo stabilizacijo in izolacijo v obliki stabilne kristalinične snovi. Glede na nedavno odkritje, da je halolaktolni prekurzor aldehida **1** mogoče pripraviti na popolnoma stereoselektiven encimatski način, rezultati te raziskave omogočajo trdno osnovo za prvo pripravo statinov preko laktonske stranske verige. Preliminarni rezultati Wittigove reakcije z modelnim ilidom so prikazani in so obetajoči. Vredno je omeniti, da so statini zdravila za zniževanje ravni holesterola, s tržno vrednostjo v letu 2008 večjo od 30 milijard ameriških dolarjev (*OK41.* Z. Časar, J. Košmrlj, *Synlett* 2009, 1144). V okviru industrijskega projekta smo skupaj s farmacevtsko tovarno Krka d.d. razvili industrijsko uporabno sintezno pot za pripravo farmacevtske učinkovine montelukast (gl. patentno prijavo: D. Kidemet, P. Benkič, A. Kljajić, B. Štefane, *Application No. 09165400.4–2117*. München: European Patent Office, 3. 9. 2009).

V sodelovanju s francoskimi partnerji smo raziskovali selektivne pretvorbe organskih molekul, katalizirane s kovinami prehoda. Pokazano je bilo, da je paladijev acetat v zelo nizkih koncentracijah (0.01−0.1 mol%) in brez liganda na paladiju zelo učinkovit katalizator za direktno ariliranje heteroaromatskih sistemov preko aktivacije C−H vezi na heteroaromatu. Pri visokih temperaturah in v polarnih organskih topilih paladijev acetat tvori Pd(0)-koloidne delce ali Pd-nanodelce, ki z aril bromidi dajejo komplekse, ki sodelujejo pri običajnih mehanizmih Heckove ali Suzuki reakcije. Na ta način smo z elektronsko revnimi in nekaterimi elektronsko bogatimi aril- in heteroaril bromidi selektivno funkcionalizirali tiofene (*OK18.* J. Roger, F. Požgan, H. Doucet, *Green Chem.* 2009, *11*, 425), furane (*OK20.* J. J. Dong, J. Roger, F. Požgan, H. Doucet, *Green Chem.* 2009, *11*, 1832) in tiazole (*OK31.* J. Roger, F. Požgan, H. Doucet, *J. Org. Chem.* 2009, *74*, 1179). Omenjena metoda je pomembna z vidika atomske ekonomičnosti, saj uporablja zelo majhne koncentracije katalizatorja in zmanjša število sintetskih stopenj, potrebnih za pripravo takšnih ariliranih derivatov. Klasične metode pripajanja namreč uporabljajo organokovinske reagente katerih priprava zahteva več stopenj, njihove reakcije pa lahko vodijo do neželenih stranskih produktov. Raziskovali smo tudi C−H aktivacijo v prisotnosti Ru-katalizatorjev. Odkrili smo, da je (*p*-cimen)rutenijev diacetat v prisotnosti $K_2CO_3$ odličen katalizator za funkcionalizacijo *orto* C−H vezi 2-piridilbenzena (*OK6.* F. Požgan, P. H. Dixneuf, *Adv. Synth. Catal*. 2009, *351*, 1737). Kvantitavno *orto*-ariliranje z neaktiviranimi arilkloridi lahko dosežemo že po 1 uri, kar kaže na izjemno aktivnost tega katalitskega sistema. Diariliranje 2-piridilbenzena z 2-halopiridini in 2- ali 3-halotiofeni pa je primerno za pripravo potencialnih tridentatnih ligandov.

V sklopu raziskav na področju novih molekularnih sond za raziskave sprememb v centralnem živčnem sistemu smo primerjali lastne rezultate z rezultati drugih raziskovalnih skupin o možnostih zasledovanja bolezenskih procesov v živih možganih. Primerjali smo uporabnost različnih molekularnih sond za raziskave tvorbe proteinskih agregatov v možganih bolnikov z Alzheimerjevo boleznijo s pozitronsko emisijsko tomografijo (*OK1.* J. R. Barrio, N. Satyamurthy, S.-C. Huang, A. Petrič, G. W. Small, V. Kepe, *Acc. Chem. Res.* 2009, *42*, 842). Sintetizirali smo vrsto analogov spojine vodnice DDNP, pri katerih je preko etilidenske verige na skelet vezan dodaten aromatski oziroma heteroaromatski obroč. Na ta način smo povečali možnost za hidrofobne interakcije s proteinskimi agregati. Pripravljene spojine smo kemijsko okarakterizirali in izmerili optične lastnosti (*OK4.* A. Žabjek, J. R. Barrio, A. Petrič, *Acta Chim. Slov.* 2009, *56*, 643). Raziskali smo tudi možnost uporabe molekularne sonde [$^{18}$F]-FDDNP v PET za in vivo slikanje sprememb v možganih pacientov z Gerstmann-Streussler-Scheinkerjevo boleznijo (GSS), pri kateri nastopa dedna nevrodegenerativna sprememba z izločanjem amiloidnih agregatov. Ugotovili smo, da je [$^{18}$F]-FDDNP PET primerna metoda za detekcijo prionskih proteinskih agregatov in ponuja možnost za spremljanje napredovanja bolezni in terapevtskih posegov (*OK11.* V. Kepe, B. Ghetti, M. R. Farlow, M. Bresjanac, K. Miller, S.-C. Huang, K.-P. Wong, J. R. Murrell, P. Piccardo, F. Epperson, G. Repovš, L. Šmid, A. Petrič, P. Siddarth, J. Liu, N. Satyamurthy, G. W. Small, J. R. Barrio, *Brain Pathol.* 2009, 419).

Naše raziskave so prispevale nova znanja na področju sinteze kompleksnih spojin, predvsem sinteze novih tipov gradnikov, in na področju razvoja novih sinteznih metod, vključno s heterogeno kemoselektivno sintezo. Nove reakcije organske sinteze smo temeljito raziskali in razložili; sintetizirali smo 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

### PLENARNA IN VABLJENA PREDAVANJA

Izvedli smo več predavanj na mednarodnih konferencah, univerzah in inštitutih.

### DRUGE DEJAVNOSTI

M. Kočevar je Nacionalni predstavnik v odboru (komiteju) Organic and Biomolecular Chemistry Division (III) IUPAC (za obdobje 2008−2009) in član upravnega odbora COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011).

*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−).

# RESEARCH PROGRAMME REPORT

## PROGRAMME GOALS

Our research programme focuses on the development of syntheses of target molecules for scientific purposes and their application, with emphasis on eco-friendly conditions (green chemistry), and high atom economy.

The programme is tightly intertwined with several international programmes from EU and USA, as well as with academic institutions from Slovenia (UL Faculty of Medicine, UL Faculty of Pharmacy, National Institute of Chemistry) and industrial research institutions (Krka, Lek). Our research efforts in 2009 were directed into developing new synthetic methods, reagents, and reactions to provide access to compounds with targeted biological activities. Assist. Prof. B. Štefane started his postdoctoral training in USA in 2009.

## RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

In the field of unsaturated cyclic amino acid derivatives we investigated the double Diels−Alder cycloaddition reaction of 2*H*-pyran-2-ones with *N*-substituted maleimides or maleic anhydride yielding bicyclo[2.2.2]octene derivatives. We observed an unusual effect of the size of the ring fused to 2*H*-pyran-2-ones on the *exo/endo* selectivity of this cycloaddition reaction. With subtle variations of starting compounds and reaction conditions (reactions under conventional heating conditions in refluxing toluene, decalin or tetralin and microwave-assisted reactions in solvents or as neat reactions) exclusively *exo*,*exo* or *exo*,*endo* products can be prepared (*OK34.* K. Kranjc, F. Perdih, M. Kočevar, *J. Org. Chem.* 2009, *74*, 6303). On the basis of our results in this field we prepared a review article describing ring transformations of 2*H*-pyran-2-ones and fused pyran-2-ones with nucleophilic reagents (*OK55.* F. Požgan, M. Kočevar, *Heterocycles* 2009, *77*, 657). Furthermore, we described a new and expeditious transformation of 5-acyl-2*H*-pyran-2-ones with various amidines as 1,3-binucleophiles into isomerically-pure (*E*)-α,β-didehydro-α-amino acid derivatives containing the 5-pyrimidyl moiety at the β-position. The procedure was performed in ethanolic (or ethanol/water) solutions in the presence of $Na_2CO_3$ as a non-toxic base and under microwave-assisted conditions. When starting from the 5-ethoxycarbonyl-2*H*-pyran-2-one derivative and in the presence of DBU as a base, the corresponding pyrano[2,3-*d*]pyrimidines were prepared. This transformation represents a new method for the synthesis of novel types of unsaturated amino acid derivatives as potential intermediates for the preparation of novel amino acids (*OK49.* J. Hren, F. Požgan, A. Bunič, V. I. Parvulescu, S. Polanc, M. Kočevar, *Tetrahedron* 2009, *65*, 8216). The above intermediates have been used as substrates for developing a new method for chemoselective hydrogenation of C=C double bonds. The catalysis, based on nano particles, is a rapidly evolving research field; currently the most important aspects are methods of green chemistry. The methods, based on the combination of supercritical carbon dioxide and ionic liquids as the reaction media, have just appeared. We reported a method for the generation and entrapment of rhodium nanoparticles in simple solid ammonium salts (not considered as ionic liquids) by exploiting their $CO_2$ induced depressed melting to yield ionic liquids. The method starts from quaternary ammonium halides or other salts ($R_4N^+X^-$), rhodium compounds ($[Rh(acac)(CO)_2]$, $RhCl_3$) with hydrogen and carbon dioxide mixed in a stainless-steel high-pressure reactor. The matrix-embedded nanoparticles thus prepared contain defined particle sizes of homogenously dispersed clusters within the range of 1−4 nm which were used as selective catalysts for the hydrogenation of simple substrates (cyclohexene and benzene) and also for more challenging β-heteroaryl-α,β-didehydro-α-amino acid derivatives (DDAAD) that cannot be easily hydrogenated by standard conditions. The new catalytic systems have exhibited a significantly distinct behaviour and selectivity (C=C double bond vs. phenyl group) toward DDAAD as compared with standard homogeneous or heterogeneous catalysts. Moreover, the catalysts can be readily separated and recycled from the reaction mixtures (*OK7.* V. Cimpeanu, M. Kočevar, V. I. Parvulescu, W. Leitner, *Angew. Chem. Int. Ed.,* 2009, *48*, 1085).

The above research work is a continuation of our systematic investigations within the project group COST D24 "Synthesis and Application of New Ligands for Asymmetric Heterogeneous Catalysis (D24/0007/02)" where a partner from Germany (Prof. Walter Leitner) was attracted. It is important to mention that Prof. Leitner was awarded the Wöhler Prize for present results from GDCh for outstanding achievements in chemistry in 2009 "for processes that conserve resources" (See: *Angew. Chem. Int. Ed.* 2009, *48*, 6587).

The reactivity of $BF_2$-complexes with 1,3-dicarbonyl ligands has been investigated. The explored synthetic strategy allows for a straightforward approach to a variety of 3-aryl and heteroarylaldehydes and ketones (*OK45.* B. Štefane, S. Polanc, *Tetrahedron* 2009, *65*, 2339). In collaboration with the Faculty of Pharmacy we synthesised a series of compounds possessing AKR1C1 and AKR1C3 enzyme inhibition (*OK14.* B. Štefane, P. Brožič, M. Vehovc, T. Lanišnik-Rižner, S. Gobec, *Eur. J. Med. Chem.* 2009, *44*, 2563). Additionally, we were able to identify the leading compound of a heterocyclic structure having the MurF inhibitory activity. The enzyme mentioned is a member of the family of enzymes responsible for the synthesis of bacterial cell wall (*OK27.* I. Sosič, B. Štefane, A. Kovač, S. Turk, D. Blanot, S. Gobec, *Heterocycles* 2010, *81*, 91).

An efficient method for the synthesis of pyrazol-3-ones involves intramolecular amination of the appropriate diazenes (*OK50.* B. Burja, M. Kočevar, S. Polanc, *Tetrahedron* 2009, *65*, 8690). This approach is a general method for the preparation of pyrazol-3-ones starting from easily available propenoic acids. The latter are prepared by the Perkin reaction of arylacetic acids with aromatic aldehydes and then transformed into corresponding hydrazides. Oxidation of the hydrazides gave the diazenes that can cyclize to pyrazol-3-ones upon treatment with $ZrCl_4$. The methoxycarbonyl protection of the N–1 of the pyrazolone derivatives is removed under mild reaction conditions. The methodology described works equally well with 3-substituted and 2,3-disubstituted propenoic acids which may open an interesting entry to a number of the pyrazolo-fused derivatives of biologically active organic compounds.

Our recent discoveries in the field of diazenes and other related research are presented in the article published in *Synlett* (*OK42.* J. Košmrlj, M. Kočevar, S. Polanc, *Synlett* 2009, 2217). Namely, the diazenes are easily available nitrogen electrophiles that can serve as convenient reagents for the production of nitrogen-containing compounds. This article focuses on four types of diazenes: dialkyl diazenedicarboxylates (previously called dialkyl azodicarboxylates), alkyl or arylaminocarbonyldiazenecarboxylates, diazenedicarboxamides (sometimes called azodicarboxamides), and diazenecarboxamides (known also as azocarboxamides). The article covers various transformations with an exception of the Diels−Alder and the Mitsunobu reactions. The aim of the research was to demonstrate the usefulness and versatility of these diazenes for synthetic purposes. The title compounds are described as convenient building blocks that enable a simple and selective introduction of nitrogen functionality into a variety of organic molecules. Electrochemical properties and biochemical aspects of the above mentioned diazenes are also described.

In collaboration with the Faculty of Pharmacy UL, the University of Warwick and the University of Leeds we have designed and synthesized novel small-molecule inhibitors of VanA and DdlB with $IC_{50}$ values in micromolar range. The results show that a phosphate group attached to the hydroxyl group of the hydroxyethylamine isostere is essential for the inhibitory activity against both VanA and DdlB. The compounds designed represent an important starting point for further optimization and modifications, to improve these inhibitory activities against VanA and DdlB. These types of inhibitors have the potential to be developed into drugs that would reverse bacterial resistance to vancomycin. Furthermore, the potency of these compounds against both VanA and DdlB suggest that it could be possible to develop broad-spectrum antimicrobials that target both Gram-negative and Gram-positive infections (*OK10.* M. Sova, G. Čadež, S. Turk, V. Majce, S. Polanc, S. Batson, A. Lloyd, D. I. Roper, C. W. Fishwick, S. Gobec, *Bioorg. Med. Chem. Lett.* 2009, *19*, 1376).

In cooperation with Lek Pharmaceuticals d.d. we have developed a synthesis of 3-acetamido-β-resorcylic acids as potential platensimycin analogues as well as FabF and FabH inhibitors. Platensimycin isolated from *Streptomyces platensis* was found to be an antibiotic, targeting highly conserved bacterial FabF enzymes involved in the biosynthesis of fatty acid. Our method consists of a simple two-step strategy and avoids the use of protecting-groups chemistry. It starts from 2-aminoresorcinol, which is first *N*-acylated and then subjected to a modified Kolbe–Schmitt carboxylation using DMSO as a solvent and $K_2CO_3$ as a base to yield the desired 3-acetamido-β-resorcylic acids. This synthetic strategy allows the preparation of a library of compounds for potential FabF and FabH inhibitors screening (*OK39*. N. Maraš, P. Štefanič Anderluh, U. Urleb, M. Kočevar, *Synlett* 2009, 437). We have also developed the first synthesis of (4*R*,6*S*)-4-(*tert*-butyldimethylsilyloxy)-6-formyltetrahydro-2*H*-pyran-2-one (aldehyde **1**) and demonstrated its value as a highly attractive precursor for the synthesis of statins via lactonized side-chain. Aldehyde **1** was prepared in its hydrated form (carbonyl water adduct), which enabled its stabilization and isolation as a stable crystalline solid. Powered by the recent discovery on highly stereoselective enzymatic synthesis of halolactole precursors, these results lay down foundations for the first formation of statins with lactonized statin side chain. Preliminary results of Wittig reaction with a model phosphonium ylide are highly encouraging. It is noteworthy that statins are cholesterol-lowering drugs holding a market value of more than US$30 billion in 2008 (*OK41*. Z. Časar, J. Košmrlj, *Synlett* 2009, 1144). Furthermore, collaboration on the industrial project with Krka Pharmaceuticals d.d. resulted in the development of an industrially applicable synthetic method for the synthesis of active substance montelukast (See patent application: D. Kidemet, P. Benkič, A. Kljajić, B. Štefane, *Application No. 09165400.4–2117*. Munich: European Patent Office, 3. 9. 2009).

In collaboration with French partners we investigated selective transformations of organic molecules catalyzed by transition metals. It was demonstrated that ligand-free palladium acetate at low loadings (0.01−0.1 mol%) can be used as a catalyst in direct arylation of heteroaromatic systems via C−H bond activation on heteroaromate. At elevated temperatures and in polar organic solvents, Pd(0)-colloids or Pd-nanoparticles are formed when palladium acetate is used as a catalyst precursor. These Pd-particles combined with aryl bromide give complexes that undergo the usual steps of the Heck or Suzuki reaction mechanisms. By this method, tiophenes (*OK18.* J. Roger, F. Požgan, H. Doucet, *Green Chem.* 2009, *11*, 425), furans (*OK20.* J. J. Dong, J. Roger, F. Požgan, H. Doucet, *Green Chem.* 2009, *11*, 1832) and thiazoles (*OK31.* J. Roger, F. Požgan, H. Doucet, *J. Org. Chem.* 2009, *74*, 1179) were selectively functionalized with electron-poor and some electron-rich aryl- and heteroaryl bromides. This method is important for atom-economy reasons due to very low loadings of catalyst and reduced number of synthetic steps to prepare such arylated derivatives. Namely, traditional cross-couplings use organometallic reagents which are usually prepared by multi-step synthesis and can lead to unwanted side-products. The C−H bond activation in the presence of Ru-catalysts was also investigated. It was demonstrated that (*p*-cymene)ruthenium diacetate in the presence of $K_2CO_3$ acts as an excellent catalyst for *ortho* C–H bond functionalisation of 2-pyridylbenzene (*OK6.* F. Požgan, P. H. Dixneuf, *Adv. Synth. Catal.* 2009, *351*, 1737). The quantitative *ortho*-arylation with unactivated aryl chlorides can be reached within one hour, showing the unprecedented activity of this catalytic system. The diarylation of 2-pyridylbenzene with 2-halopyridines and 2- or 3-halothiophenes led to the potential tridentate ligands.

Investigations of new molecular probes for detecting changes in the central nervous system (CNS) were published as a comparison of our own work and the results of other research groups on *in vivo* methods for the assessment of disease progression. We compared different molecular probes used by Positron Emission Tomography (PET) to assess the formation of protein aggregates in the CNS of Alzheimer's disease patients (*OK1.* J. R. Barrio, N. Satyamurthy, S.-C. Huang, A. Petrič, G. W. Small, V. Kepe, *Acc. Chem. Res.* 2009, *42*, 842). We prepared and characterized a series of analogs of the lead compound DDNP with an aromatic or heteroaromatic ring linked to the parent molecule via an ethylidene tether. The introduced aromatic/heteroaromatic ring offers an additional opportunity for the interaction between the molecule and protein aggregates (*OK4.* A. Žabjek, J. R. Barrio, A. Petrič, *Acta Chim. Slov.* 2009, *56*, 643). We have investigated the applicability of molecular probe [$^{18}$F]-FDDNP with PET for in vivo imaging of the changes in the CNS of Gerstmann-Streussler-Scheinker (GSS) disease patients, a familial neurodegenerative brain disorder. In the CNS of GSS patients amyloid protein aggregates separate. We have found that [$^{18}$F]-FDDNP PET is a feasible method for detecting prion protein accumulation in living patients, and that it presents a way for monitoring the progression of the disease and monitoring therapeutic interventions (*OK11.* V. Kepe, B. Ghetti, M. R. Farlow, M. Bresjanac, K. Miller, S.-C. Huang, K.-P. Wong, J. R. Murrell, P. Piccardo, F. Epperson, G. Repovš, L. Šmid, A. Petrič, P. Siddarth, J. Liu, N. Satyamurthy, G. W. Small, J. R. Barrio, *Brain Pathol.* 2009, 419).

Our research has generated 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, including heterogeneous chemoselective syntheses. Novel reactions in organic synthesis have been thoroughly investigated and explained; on the other hand, we have also synthesized some new biologically active compounds. Some of our compounds thus prepared were shown to be suitable for detecting certain diseases.

## OTHER RELEVANT ACHIEVEMENTS

### PLENARY AND INVITED LECTURES

Several lectures were delivered at international conferences, universities and institutes.

### OTHER ACTIVITIES

M. Kočevar was acting as a National Representative of IUPAC Organic and Biomolecular Chemistry Division (III) Committee (for the period 2008−2009) and is a member of the Management Committee COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011).

*Editorial activities:* K. Kranjc has been a member of the editorial board (2007−) of the *Acta Chimica Slovenica* (ACSi), M. Kočevar is a member of editorial board of *Periodica polytechnica. Chemical engineering* (2003−), and S. Polanc is a member of editorial board of the *Topics in heterocyclic chemistry* (2008−).

# KEMIJSKO INŽENIRSTVO
## CHEMICAL ENGINEERING

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**P2–0191**

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# 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 določamo 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

Mikroenkapsulacija 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 mikroenkapsulacijo 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 mikroenkapsulacije 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 izdelava 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
- Diskretno modeliranje delovanja kolone z mehurčki v prisotnosti ne-newtonskega medija
- Eksperimentalni študij hidrodinamskih in kinetično-adsorpcijskih parametrov kolone z ekspandiranim slojem
- Izolacija aktivnih farmacevtskih učinkovin
- Reološko kompleksne tekočine

*Polimerno inženirstvo:*

- Raziskave na področju mikroenkapsulacije
- 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 formaldehidnih 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
- Testiranje 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

# ZNANSTVENI DOSEŽKI

## MIKROREAKTORSKA TEHNOLOGIJA V PROCESNEM INŽENIRSTVU

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 svojih raziskav smo preučili različne homogene in heterogene biokatalitske sisteme v mikroreaktorjih ter jih primerjali z literaturnimi podatki za izvedbe procesov v klasičnih reaktorjih. Objava v preglednem znanstvenem članku:

*POHAR, Andrej, PLAZL, Igor. Process intensification through microreactor application. Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 537–544.*

## ADSORPCIJA VANKOMICINA NA AMBERLIT XAD-16

Za določitev adsorpcijske kapacitete smo najprej pridobili ravnotežne podatke vankomicina na polimerni smoli Amberlite XAD-16. Eksperimentalni podatki so se najbolj skladali z Langmuirjevo adsorpcijsko izotermo, pri kateri znaša maksimalna kapaciteta 53,76 kg/m$^3$ smole pri pH 7. Raziskave smo nadaljevali v laboratorijski koloni s strnjenim in ekspandiranim slojem adsorbenta. Dinamiko procesa smo opisali s pomočjo prebojnih krivulj, napovedanih z enostavnim matematičnim modelom, ki upošteva tudi aksialno disperzijo. Primerjava eksperimentalnih in napovedanih rezultatov in narejene parametrične občutljivosti je omogočila boljše razumevanje procesa z namenom optimizacije v večjem merilu. Učinkovitost adsorpcije v ekspandiranem sloju je povsem primerljiva z učinkovitostjo strnjenega sloja. Tako je adsorpcija v ekspandiranem sloju dobra alternativa klasični izolaciji vankomicina iz fermentacijske brozge. Rezultati so bili objavljeni v članku:

*BORIN, Bojan, PAVKO, Aleksander. Adsorption of Vancomycin on Amberlite XAD-16 in a packed bed column, Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 479–483.*

## RAZVOJ 2-PARAMETRSKEGA DISKRETNEGA MODELA KOLONE Z MEHURČKI

V skladu s programom je razvit dvo-parametrski celični model z reciklom, ki bi kot stopenjski model ustrezal popisu dogajanja toka v kolonah z mehurčki ob prisotnosti ne-newtonskga medija z izrazito elastičnimi lastnostmi. Pri iskanju orientacijskih vrednosti nenastavljivih parametrov in realnih vrednosti obratovalnih parametrov smo se naslanjali na izsledke predhodnih študij. Rezultati simulacije so pokazali, da je pri večjem številu zaporednih mešalnih celic uvedeni recikel uspešno blažil skoraj čepasti tok v koloni. *Celični model z reciklom* se pri srednji stopnji povratnega mešanja in srednji vrednosti $k_La$ dobro ujema z aksialno disperznim modelom. Primerjava izračunanih koncentracijskih profilov razvitega modela s kvalitativnimi testi z barvnim sledilcem na koloni z ne-newtonskim medijem kaže na primernost razvitega modela pri evalvaciji volumetričnega koeficienta snovnega prestopa na osnovi pravilno organiziranih eksperimentalnih meritev.

## SUSPENZIJSKA POLIMERIZACIJA ZA SINTEZO MIKROSFERNIH NA PRITISK OBČUTLJIVIH AKRILATNIH LEPIL

Preučevali smo vpliv molekulske mase polimera in vpliv reakcij zamreževanja na adhezivne lastnosti mikrosfernih na pritisk občutljivih akrilatnih lepil. Sintetizirali smo nanokompozitna mikrosferna na pritisk občutljiiva akrilatna lepila z uporabo modificiranih montmorilonitnih glin. Preučili smo vpliv modifikacije gline in vpliv količine uporabljenega nanopolnila na adhezivne in viskoelastične lastnosti lepil. Rezultati raziskav so objavljeni v člankih:

*KAJTNA, Jernej, GOLOB, Janvit, KRAJNC, Matjaž. The effect of polymer molecular weight and crosslinking reactions on the adhesion properties of microsphere water-based acrylic pressure-sensitive adhesives. Int. j. adhes. adhes. 2009, vol. 29, no. 2, pp. 186–194.*

*KAJTNA, Jernej, ŠEBENIK, Urška. Microsphere pressure sensitive adhesives – acrylic polymer/montmorillonite clay nanocomposite materials. Int. j. adhes. adhes. 2009, vol. 29, no. 5, pp. 543–550.*

## KINETIKA ZAMREŽEVANJA ELASTOMEROV Z ORGANSKIMI PEROKSIDI IN RAZISKAVE MORFOLOGIJE ELASTOMERNIH NANOKOMPOZITOV TER MODELIRANJE NJIHOVIH DINAMIČNIH MEHANSKIH LASTNOSTI

Simulirali smo kinetiko zamreževanja elastomera z organskimi peroksidi. Modelirali smo dinamične mehanske lastnosti HNBR kavčuka ojačanega s koagenti ter preučevali morfologijo disperzije koagentov v elastomerni matrici. Rezultati raziskave so objavljeni v člankih:

*LIKOZAR, Blaž, KRAJNC, Matjaž. Simulation of chemical kinetics of elastomer crosslinking by organic peroxides. Polym. eng. sci., 2009, vol. 49, no.1, pp. 60–72.*

*LIKOZAR, Blaž, KRAJNC, Matjaž. Modeling of the dynamic mechanical properties of the coagent reinforced row hydrogenated poly(butadiene-co-acrylonitrile) (HNBR) and the morphology of coagent nanodispersions in HNBR matrix. Polimery, 2009, vol. 54, no. 6, pp. 32–43.*

## POLIMERNI NANOKOMPOZITI

S pomočjo polimerizacije v masi in s pomočjo mešanja v talini smo pripravili polimetilmetakrilatne nanokompozite. Kot nanopolnilo smo uporabili modificiran montmorilonit. Primerjali smo lastnosti nanokompozitov pridobljenih z omenjenima postopkoma. Rezultati raziskave so objavljeni v članku:

*KRAJNC, Matjaž, ŠEBENIK, Urška. Poly(methyl methacrylate)/montmorillonite nanocomposites prepared by bulk polymerization and melt compounding. Polym. compos., 2009, vol. 30, no. 11, pp. 1678–1686.*

## POLISILOKSANSKE EMULZIJE

Raziskovali smo termično stabilnost in kinetiko termičnega razpada polisiloksanske emulzije. Z uporabo izokonverzijske metode in z uporabo integralnega postopka, smo na osnovi rezultatov dinamične termogravimetrične analize, določili kinetiko termičnega razpada polisiloksanske emulzije pri izotermnih pogojih in v območju temperatur, ki se uporabljajo v industriji visokotlačnega litja aluminijevih zlitin. Rezultati raziskave so objavljeni v članku:

*MOHORIČ, Ines, KRAJNC, Matjaž, ŠEBENIK, Urška. Model-free kinetics analysis of thermal degradation of polysiloxane lubricant. Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 493–496.*

## MIKROREAKTORSKA TEHNOLOGIJA V BIOKEMIJSKEM INŽENIRSTVU

Na področju mikroreaktorske tehnologije smo nadaljevali študije homogenih in heterogenih biokatalitskih sistemov. Teoretično in eksperimentalno smo preučili encimsko katalitsko sintezo izoamil acetata v kontinuirno delujočem mikroreaktorju. Proces esterifikacije izoamil alkohola in ocetne kisline poteka na medfazni površini paralelnega toka heksana in vodne faze z raztopljeno lipazo. 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 Ping-Pong Bi-Bi mehanizmom. Eksperimentalni podatki, ki se dobro ujemajo z teoretičnimi napovedmi, so pokazali 35 % konverzijo pri zadrževalnem času 36,5 sek in 45 ºC, pri 0,5 M vstopni koncentraciji obeh reaktantov. Študij encimsko katalizirane sinteze izoamil acetata smo nadaljevali v dvofaznem sistemu ionske tekočine 1-butil-3-metilpiridinijev dicianamid/n-heptan v ψ-oblikovanem mikroreaktorju. Izbran dvofazni sistem z raztopljeno lipazo B omogoča učinkovito katalitsko reakcijo s sočasno ekstrakcijo produkta v n-heptan. Pri predhodno določenih procesnih pogojih je prišlo do nastajanja 48.4 $g/m^3s$ produkta, kar je skoraj trikrat bolje kot v intenzivno mešanem šaržnem sistemu. Razlog za tako učinkovit proces je v glavnem v izredno učinkoviti reakcijsko difuzijski dinamiki mikroreaktorja, kjer prihaja do razvoja tokovnega profila z veliko medfazno površino za reakcijo in sočasno ekstrakcijo produkta. Od homogenih sistemov smo študirali še encimsko katalizirano oksidacijo aminokisline L-DOPA v mikroreaktorju pri različnih pogojih nasičenosti vodne faze s kisikom. Rezultati raziskav so objavljeni v treh člankih:

*ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Modelling and experimental studies on lipase-catalyzed isoamyl acetate synthesis in a microreactor. Process biochem., 2009, vol. 44, no. 10, pp. 1115–1121.*

*POHAR, Andrej, PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. Lipase-catalyzed synthesis of isoamyl acetate in an ionic liquid/n-heptane two-phase system at the microreactor scale. Lab chip, 2009, vol. 9, no. 23, pp. 3385–3390.*

*TIŠMA, Marina, ZELIĆ, Bruno, VASIĆ-RAČKI, Đurđa, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Modelling of laccase-catalyzed L-DOPA oxidation in a microreactor. Chem. eng. j., 2009, vol. 149, no. 1/3, pp. 383–388.*

## VPLIV ENCIMSKE OBDELAVE VLAKNIN NA MEHANSKE LASTNOSTI IN MORFOLOŠKE KARAKTERISTIKE VLAKNIN

Biotehnologija ponuja industriji celuloze in papirja številne priložnosti za dosego ključnih ciljev trajnostnega razvoja, od zmanjšanja porabe energije in s tem količine odpadnih plinov pri izgorevanju fosilnih goriv, do znižanja koncentracije organskih snovi v odpadnih vodah. V svojih raziskavah smo proučili vpliv encimske obdelave vlaknin, uporabljanih v Papirnici Vevče, na mehanske lastnosti in morfološke karakteristike vlaknin, vključno s sleditvijo razgradnje trahej. V laboratorijskem merilu smo pri različnih procesnih pogojih testirali nekatere komercialne encime (celulaze in ksilanaze ter njihove mešanice) ter opredelili potencialne prihranke energije na osnovi zmanjšanja intenzivnosti mehanske obdelave (mletja) potrebne za dosego želenih lastnosti vlaken. Rezultati raziskave so objavljeni v članku:

*ŽNIDARŠIČ PLAZL, Polona, RUTAR, Vera, RAVNJAK, David. The effect of enzymatic treatments of pulps on fiber and paper properties. Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 497–506.*

### FARMACEVTSKE UČINKOVINE VIŠJIH GLIV. PRODUKCIJA IN IZOLACIJA FARMACEVTSKO AKTIVNIH UČINKOVIN GLIVE *GRIFOLA FRONDOSA*

Raziskave so potekale v treh smereh: (1) submerzna kultivacija v mešalnem bioreaktorju v tekočem gojišču, kjer smo se osredotočili na postopke optimizacije za produkcijo biomase ter farmacevtrsko aktivnih snovi ter izdelali nov postopek kultivacije na osnovi flotacije in imobilizacije glivine biomase na stenah bioreaktorjev; (2) izdelali smo postopek sterilizacije in kultivacije aktivne glivine biomase na koruzni slami – sekundarnih surovinah agroživilske in lesne industrije; (3) nadaljevali smo raziskave optimizacije kultivacije gob *Grifola frondosa* na pilotnem nivoju na eksperimentalni farmi gob. Dosežki so dokumentirani v treh člankih:

*HABIJANIČ, Jožica, ŠVAGELJ, Mirjan, BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Submerged and solid-state cultivation of bioactive extra- and intracellular polysaccharides of medicinal mushrooms Ganoderma lucidum (W. Curt.: Fr.) P. Karst. and Grifola frondosa (Dicks.: Fr.) S. F. Gray (Aphyllophoromycetideae). Int. j. medic. mushrooms, 2009, vol. 11, no. 4, pp. 409–418.*

*SCHWAB, Karima, BADER, Johannes, BROKAMP, Christian, POPOVIĆ, Milan K., BAJPAI, Rakesh K., BEROVIČ, Marin. Dual feeding strategy for the production of [alpha]-amylase by Bacillus caldolyticus using complex media. New biotechnology, 2009, vol. 26, no. 1/2, pp. 68–74.*

*GREGORI, Andrej, ŠVAGELJ, Mirjan, BEROVIČ, Marin, LIU, Y., ZHANG, Jingsong, POHLEVEN, Franc, KLINAR, Dušan. Cultivation and bioactivity assessment of Grifola frondosa fruiting bodies on olive oil press cakes substrates. New biotechnology, pp. 1–3, doi: 10.1016/j.nbt.2009.08.001.*

### NITRIFIKACIJA V BIOLOŠKEM REAKTORJU S PRITRJENO BIOMASO

Študirali smo vpliv dveh različnih nosilcev na proces nitrifikacije v biološkem reaktorju s pritrjeno biomaso. Testirana nosilca sta bila klasični cilindrični polietilenski obroč (AnoxKaldnes) in sferični nosilec gelskega tipa na osnovi polivinil alkohola (Kuraray, PVA-gel carrier). Rezultati raziskave so objavljeni v članku:

*LEVSTEK, Meta, PLAZL, Igor. Influence of carrier type on nitrification in the moving-bed biofilm process. Water sci. technol., 2009, vol. 59, no. 5, pp. 875–882.*

## 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 requires detailed knowledge of complex transport mechanisms. These research contents enable an integrated multidisciplinary systematic approach, the development of fundamental chemical engineering science knowledge and its application in the specific fields or branches of chemical engineering. Programme goals have been defined in accordance with the division to the specific branches of chemical engineering, which are: *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 in fine chemical/pharmaceutical industries about 50% of reactions could benefit from 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 proper 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 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 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, defining the appropriate viscous model, which takes into account the low and high shear rate behaviour of blood, is essential. During 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, which 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 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 aggressively 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 many 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 studied. The research 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 foams production.

The kinetics of vulcanization process and heat transfer during vulcanization process for selected rubber blends was 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.

## 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 production. 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 however 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 like 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 is 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 being investigated. The main goal is to obtain new knowledge about the fungal and enzyme applicability in solving problems of industrial organic waste effluents with bioremediation by environmentally friendly technology. From the economical point of view 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
- Discrete modelling of bubble column in the presence of non-Newtonian liquid
- Experimental study of hydrodynamics and kinetic/adsorption parameters of expanded-bed column
- Isolation of active pharmaceutical agents
- Rheologicaly complex fluids

*Polymer engineering:*

- Microencapsulation research
- Synthesis, characterization and optimization of the synthesis process of acrylic adhesives
- Synthesis, characterization and optimization of the synthesis process of nanocomposite materials
- Synthesis, characterization and optimization of the synthesis process of polysiloxane emulsions
- Synthesis, characterization and optimization of the synthesis process of formaldehyde resins
- Research and development of a technology for melamine foams production
- 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 industries
- Isolation and purification of extra and intracellular fungal polysaccharides
- In-vitro testing of immunostimulatory activities of isolates by induction of cytokines in human peripheral mononuclear blood cells (PBMC)

*Environmental engineering*

- Research in the field of bioremediation
- Nitrification in the moving-bed biofilm process

## SCIENTIFIC ACHIEVEMENTS

### MICROREACTOR TECHNOLOGY IN PROCESS ENGINEERING

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 biocatalytic systems were studied within microreactors and compared with literature data for processes in classical reactors. The achievement is published in:

*POHAR, Andrej, PLAZL, Igor. Process intensification through microreactor application. Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 537–544.*

### ADSORPTION OF VANCOMYCIN ON AMBERLITE XAD-16

The equilibrium adsorption studies of Vancomycin on Amberlite XAD-16 to determine the adsorption capacity were carried out first. The experimental data fitted best with Langmuir isotherm. Maximum capacity was $q_0 = 53.76$ kg/m$^3$ resin at pH 7. In the following step, the adsorption was studied in a laboratory packed bed and expanded bed adsorption columns. A simple mathematical model taking into account axial dispersion was applied to describe the dynamics of the process with breakthrough curves. Experimental and predicted results were compared, some parametric sensitivity analyses were made to better understand the process for large scale optimisation. The expanded-bed adsorption efficiency was observed to be comparable to that of packed-bed adsorption. Thus the expanded-bed adsorption is an appropriate alternative to the traditional process of recovery and isolation of Vancomycin. The results were published in:

*BORIN, Bojan, PAVKO, Aleksander. Adsorption of Vancomycin on Amberlite XAD-16 in a packed bed column, Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 479–483.*

## DEVELOPMENT OF TWO-PARAMETER DISCRETE MODEL OF BUBBLE COLUMN

Two-parameter cell model of bubble column was developed with a purpose to fit the nature of a specific non-Newtonian medium. The nature of discontinuous stage model proved to be suitable for an inventory of local phenomena in the column, a cell model with recycle is able to control the activity in each cell in the column. In searching for non-adjustable parameters and appropriate values of the operating parameters, we were drawing upon the results of previous studies. The column operated in a concurrent up-flow mode and was divided into four, six, ten and thirty equal-sized cells. A recycle was introduced from the last cell into the first. The results of numerical simulations prove that for a large number of successive mixing cells a recycle introduced in the model successfully mitigates the plug flow in the column. This cell model with recycle quite fits with the axial dispersion model, whenever the backmixing and the volumetric transfer coefficient (kLa) are of mean values. Comparison of simulated concentration profiles with qualitative tracer tests on a column with non-Newtonian medium demonstrates that the developed model for the evaluation of volumetric transfer coefficient on the basis of properly organized experimental measurements is suitable.

## SUSPENSION POLYMERIZATION FOR THE SYNTHESIS OF MICROSPHERE WATER-BASED ACRYLIC PRESSURE-SENSITIVE ADHESIVES

The effect of polymer molecular weight and cross linking reactions on the adhesive properties of microsphere water-based acrylic pressure-sensitive adhesives was studied. Nanocomposite microsphere water-based acrylic pressure sensitive adhesives by the use of modified montmorillonite clays were synthesized. The effect of clay modification and the effect of amount of clay used on the adhesion and viscoelastic properties were studied. The results are published in:

*KAJTNA, Jernej, GOLOB, Janvit, KRAJNC, Matjaž. The effect of polymer molecular weight and crosslinking reactions on the adhesion properties of microsphere water-based acrylic pressure-sensitive adhesives. Int. j. adhes. adhes. 2009, vol. 29, no. 2, pp. 186–194.*

*KAJTNA, Jernej, ŠEBENIK, Urška. Microsphere pressure sensitive adhesives – acrylic polymer/montmorillonite clay nanocomposite materials. Int. j. adhes. adhes. 2009, vol. 29, no. 5, pp. 543–550.*

## CHEMICAL KINETICS OF ELASTOMER CROSSLINKING BY ORGANIC PEROXIDES AND MODELLING OF THE DYNAMIC MECHANICAL PROPERTIES OF THE COAGENT REINFORCED ELASTOMERS AND THE MORPHOLOGY OF COAGENT NANODISPERSIONS IN ELASTOMER MATRIX

Chemical kinetics of elastomer crosslinking by organic peroxides was simulated. The dynamic mechanical properties of the coagent reinforced row hydrogenated poly(butadiene-co-acrylonitrile) (HNBR) were modelled and the morphology of coagent nanodispersions in HNBR matrix were studied. The results are published in:

*LIKOZAR, Blaž, KRAJNC, Matjaž. Simulation of chemical kinetics of elastomer crosslinking by organic peroxides. Polym. eng. sci., 2009, vol. 49, no.1, pp. 60–72.*

*LIKOZAR, Blaž, KRAJNC, Matjaž. Modelling of the dynamic mechanical properties of the coagent reinforced row hydrogenated poly(butadiene-co-acrylonitrile) (HNBR) and the morphology of coagent nanodispersions in HNBR matrix. Polimery, 2009, vol. 54, no. 6, pp. 32–43.*

## POLYMER NANOCOMPOSITES

Polymethyl metacrylate/montmorillonite nanocomposites were prepared by melt compounding and by bulk polymerization. The resulting nanocomposite properties obtained by different preparation processes were compared. The results are published in:

*KRAJNC, Matjaž, ŠEBENIK, Urška. Poly(methyl methacrylate)/montmorillonite nanocomposites prepared by bulk polymerization and melt compounding. Polym. compos., 2009, vol. 30, no. 11, pp. 1678–1686.*

## POLYSILOXANE EMULSIONS

Thermal degradation behaviour of dried polysiloxane emulsion used as a lubricant in die casting industry was investigated. The degradation was studied by thermal gravimetric analysis (TGA) through several non-isothermal experiments. The isoconversional kinetic analysis was applied to the non-isothermal experiments and the experimental results were processed by integral procedure which enabled activation energy determination. On the basis of determined activation energy isothermal decomposition behaviour of the lubricant at different temperatures was successfully predicted. The predictions were verified by isothermal TGA experiments. The results are published in:

*MOHORIČ, Ines, KRAJNC, Matjaž, ŠEBENIK, Urška. Model-free kinetics analysis of thermal degradation of polysiloxane lubricant. Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 493–496.*

## MICROREACTOR TECHNOLOGY IN BIOCHEMICAL ENGINEERING

A lipase-catalyzed synthesis of isoamyl acetate was studied in a continuously operated pressure-driven microreactor. The esterification of isoamyl alcohol and acetic acid occurred at the interface between n-hexane and the aqueous phase with dissolved lipase B from Candida antarctica. By adjusting the flow rates of both phases, a parallel laminar flow with liquid-liquid boundary in the middle of the microchannel could be re-established and phase separation was achieved at the y-shaped exit of the microreactor. A 3D mathematical model was developed, considering the velocity profile, convection, diffusion, and enzyme reaction terms, where the esterification rate was described with a Ping-Pong Bi-Bi mechanism and inhibition with both substrates. The experimental data, which were in good agreement with model simulations, have demonstrated 35% conversion at residence time of 36.5 sec at 45 ºC and with 0.5 M acetic acid and isoamyl alcohol inlet concentrations, which is much faster than in any literature reported so far. Furthermore, a continuously operated ψ-shaped microreactor was used for lipase-catalyzed synthesis of isoamyl acetate in 1-Butyl-3-methylpyridinium dicyanamide/n-heptane two-phase system. The chosen solvent system with dissolved Candida antarctica lipase B, which was attached to the ionic liquid/n-heptane interfacial area due to its amphiphilic properties, was shown to be highly efficient and enabled simultaneous esterification and product removal. At preliminarily selected conditions regarding the type of acyl donor, its molar ratio to alcohol and enzyme concentration, 48.4 g/m$^3$s of isoamyl acetate was produced, which was almost three times better compared to the intensely mixed batch process. This was mainly due to efficient reaction-diffusion dynamics in the microchannel system, where the developed flow pattern comprising of intense emulsification provided a large interfacial area for the reaction and simultaneous product extraction. Laccase-catalyzed L-DOPA oxidation in an oxygen-saturated water solution was studied in a y-shaped microreactor with different residence times and with different inlet concentrations of L-DOPA and oxygen. The results are published in:

*ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Modelling and experimental studies on lipase-catalyzed isoamyl acetate synthesis in a microreactor. Process biochem., 2009, vol. 44, no. 10, pp. 1115–1121.*

*POHAR, Andrej, PLAZL, Igor, ŽNIDARŠIČ PLAZL, Polona. Lipase-catalyzed synthesis of isoamyl acetate in an ionic liquid/n-heptane two-phase system at the microreactor scale. Lab chip, 2009, vol. 9, no. 23, pp. 3385–3390.*

*TIŠMA, Marina, ZELIĆ, Bruno, VASIĆ-RAČKI, Đurđa, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Modelling of laccase-catalyzed L-DOPA oxidation in a microreactor. Chem. eng. j., 2009, vol. 149, no. 1/3, pp. 383–388.*

## THE INFLUENCE OF DIFFERENT CELLULASES AND XYLANASES OR THEIR MIXTURES ON QUALITY OF DIFFERENT BLEACHED KRAFT PULPS

Biotechnological treatment of pulps provides great potential for the reduction of energy consumption and emissions of greenhouse gases. In our research we investigated the influence of different commercial cellulases and xylanases or their mixtures on the quality of different bleached kraft pulps. The effects of enzymes on the reduction of sugars release and changes in fiber length were assessed for different pulps used in Papirnica Vevče. Besides, vessel cell deformation was observed as a consequence of all enzymes applications. Furthermore, physical and mechanical properties of laboratory sheets made with enzymatically treated pulps were evaluated for various refining conditions and compared to those of untreated pulps. Potential energy savings up to 17% were achieved with enzyme treatment, while there was some decrease in pulp quality observed.

*ŽNIDARŠIČ PLAZL, Polona, RUTAR, Vera, RAVNJAK, David. The effect of enzymatic treatments of pulps on fiber and paper properties. Chem. biochem. eng. q., 2009, vol. 23, no. 4, pp. 497–506.*

## RESEARCH ON PHARMACEUTICALLY ACTIVE COMPOUNDS OF *GRIFOLA FRONDOSA*

Research on pharmaceutically active compounds of *Grifola frondosa* took place in three main directions: (1) Submerged cultivation on liquid substrate in a stirred tank reactor was optimized in relation to substrate composition as well as in the process optimization, where a new technology, based on flotation and immobilization of fungal biomass on the bioreactors walls including specific double stage feed technology for high production of active fungal biomass was developed; (2) New sterilization and cultivation procedure for the exploitation of agricultural waste secondary raw material (corn straw) was developed; (3) Optimization of solid substrates based on wheat and rye straw for cultivation of *Grifola frondosa* fruit bodies on experimental pilot plant was studied. The results are published in:

*HABIJANIČ, Jožica, ŠVAGELJ, Mirjan, BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Submerged and solid-state cultivation of bioactive extra- and intracellular polysaccharides of medicinal mushrooms Ganoderma lucidum (W. Curt.: Fr.) P. Karst. and Grifola frondosa (Dicks.: Fr.) S. F. Gray (Aphyllophoromycetideae). Int. j. medic. mushrooms, 2009, vol. 11, no. 4, pp. 409–418.*

*SCHWAB, Karima, BADER, Johannes, BROKAMP, Christian, POPOVIĆ, Milan K., BAJPAI, Rakesh K., BEROVIČ, Marin. Dual feeding strategy for the production of [alpha]-amylase by Bacillus caldolyticus using complex media. New biotechnology, 2009, vol. 26, no. 1/2, pp. 68–74.*

*GREGORI, Andrej, ŠVAGELJ, Mirjan, BEROVIČ, Marin, LIU, Y., ZHANG, Jingsong, POHLEVEN, Franc, KLINAR, Dušan. Cultivation and bioactivity assessment of Grifola frondosa fruiting bodies on olive oil press cakes substrates. New biotechnology, pp. 1–3, doi: 10.1016/j.nbt.2009.08.001.*

## NITRIFICATION IN THE MOVING-BED BIOFILM PROCESS

Two types of carriers differing fundamentally in size, shape and structure were evaluated in parallel testing for nitrification potential using the moving-bed biofilm reactor (MBBR) technology. One of the carriers used was a cylindrical high-density polyethylene ring-shaped carrier (AnoxKaldnes, K1 carrier) and the other was a spherical polyvinyl alcohol (PVA) gel bead shaped carrier (Kuraray, PVA-gel carrier). The results are published in:

*LEVSTEK, Meta, PLAZL, Igor. Influence of carrier type on nitrification in the moving-bed biofilm process. Water sci. technol., 2009, vol. 59, no. 5, pp. 875–882.*

# SEPARACIJSKI PROCESI TOPLOGREDNIH PLINOV ZA TRAJNOSTNI RAZVOJ

## SEPARATION PROCESSES OF GREENHOUSE GASES FOR SUSTAINABLE DEVELOPMENT

**PROGRAMSKA SKUPINA** / RESEARCH PROGRAMME GROUP

**P2–0346**

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# 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.

## 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

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

*Publikacije:*

- Šostarič, Maja, Golob, Janvit, Bricelj, Mihael, Klinar, Dušan, Pivec, Aleksandra, Studies on the Growth of *Chlorella vulgaris* in Culture Media with Different Carbon Sources, Chemical and biochemical engineering quarterly, Volume: 23 Issue: 4 Pages: 471–477. Published: Dec. 2009.

### RAZISKAVE INDUSTRIJSKIH PROCESOV Z NAMENOM EKOLOŠKE IN ENERGETSKE OPTIMIZACIJE

*Publikacije:*

- Zakrajšek, Nejc, Knez, Sergej, Ravnjak David, Golob, Janvit, Analysis of Modified Starch Adsorption Kinetics on Cellulose Fibers via the Modified Langmuir Adsorption Theory, Chemical and biochemical engineering quarterly, Volume: 23 Issue: 4 Pages: 461–470. Published: Dec. 2009.
- Šrekl, Jože, Golob, Janvit, Statistical Modeling in Fire-ignition Hazard Evaluation, Chemical and biochemical engineering quarterly, Volume: 23 Issue: 3 Pages: 309–315. Published: Sep. 2009.

- Zakrajšek, Nejc, Fuente, E., Blanco, A., Golob, Janvit, Influence of Cationic Starch Adsorption on Fiber Flocculation, Chemical engineering & technology, Volume: 32 Issue: 8 Pages: 1259–1265. Published: Aug. 2009.
- Zakrajšek, Nejc, Golob, Janvit, The Influence of Modified Starch on the Process Water Quality in Papermaking and the Paper Properties, Starch-Stärke, Volume: 61 Issue: 2 Pages: 109–115. Published: Feb. 2009.

### RAZISKAVE NA PODROČJU INŽENIRSTVA OKOLJU PRIJAZNIH PROIZVODOV

*Publikacije:*

- Gregori, Andrej, Švagelj, Mirjan, Berovič, Marin, Liu, Y., Zhang, Jingsong, Pohleven Franc, Klinar, Dušan, Cultivation and Bioactivity Assessment of *Grifola frondosa* fruiting bodies on olive oil press cakes substrates, New biotechnology, Volume: 26 Issue: 5 Pages: 260–262. Published: Nov. 2009.

## DRUGI RELEVANTNI DOSEŽKI

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

*Prispevki na mednarodnih konferencah:*

- Šoštarič, Maja, Selišnik, Aljaž, Knez, Sergej, Golob, Janvit, Bricelj, Mihael, Klinar, Dušan, Pivec, Aleksandra, Studies on growth of *Chlorella vulgaris* under different cultivation conditions. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.

### RAZISKAVE INDUSTRIJSKIH PROCESOV Z NAMENOM EKOLOŠKE IN ENERGETSKE OPTIMIZACIJE

*Prispevki na mednarodnih konferencah:*

- Zakrajšek, Nejc, Golob, Janvit, Knez, Sergej, Ravnjak, David, The influence of modified starch on the process water quality in the papermaking. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.
- Klofutar, Boštjan, Golob, Janvit, Klofutar, Cveto, Žagar, Ema, Poljanšek, Ida, Kinetics of the transesterification of rapeseed and waste sunflower oils. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.
- Šrekl, Jože, Golob, Janvit, New approach to calculate the probability of ignition : [lecture]. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.

## RAZISKAVE NA PODROČJU INŽENIRSTVA OKOLJU PRIJAZNIH PROIZVODOV

*Prispevki na mednarodnih konferencah:*

- Likozar, Blaž, Modeling of elastomer cross-linking by organic peroxides : correlation of kinetics, mass transfer, heat transfer and viscoelasticity. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, str. 97.
- Likozar, Blaž, Kinetic modelling of the peroxide cross-linking of polymer/monomer blends : from a theoretical model framework to its application for a complex polymer/monomer system. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, str. 98.
- Likozar, Blaž, Major, Zoltan, The influence of nitrile content, hydrogenation and compound preparation on morphological, mechanical, thermal and other properties of (hydrogenated) nitrile rubber/carbon nanotube nanocomposites. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, str. 151.
- Likozar, Blaž, Major, Zoltan, Modelling of the filled elastomer moduli of unfunctionalized, hydroxy-, and carboxy- functionalized multi-walled carbon nanotubes reinforced hydrogenated nitrile rubber and the morphology of nanocomposites. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, str. 151.
- Likozar, Blaž, Major, Zoltan, Modelling of the filled elastomer moduli of unfunctionalized, hydroxy-, and carboxy- functionalized multi-walled carbon nanotubes reinforced hydrogenated nitrile rubber and the morphology of nanocomposites. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, str. 17.
- Likozar, Blaž, Major, Zoltan, The influence of nitrile content, hydrogenation and compound preparation on morphological, mechanical, thermal and other properties of (hydrogenated) nitrile rubber/carbon nanotube nanocomposites. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, str. 18.
- Likozar, Blaž, Kinetic modelling of the peroxide cross-linking of polymer/monomer blends : from a theoretical model framework to its application for a complex polymer/monomer system. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, str. 23.
- Likozar, Blaž, Modeling of elastomer cross-linking by organic peroxides : correlation of kinetics, mass transfer, heat transfer and viscoelasticity. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, str. 24.

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 fossil fuel resources depletion are becoming the most important challenges facing 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 closing oil crisis and the dramatic climate changes, renewable, low-level carbon and economically achievable energy sources are vitally important. A relatively small part of liquid fuels consumed for transportation is nowadays 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 of carbon dioxide emissions minimization, 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

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

*Publications:*

- Šostarič M, Golob, Janvit, Bricelj Mihael, Klinar Dušan, Pivec Aleksandra, Studies on the Growth of *Chlorella vulgaris* in Culture Media with Different Carbon Sources, Chemical and biochemical engineering quarterly, Volume: 23 Issue:4 Pages: 471–477. Published: Dec. 2009.

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

*Publications:*

- Zakrajšek, Nejc, Knez, Sergej, Ravnjak, David, Golob, Janvit, Analysis of Modified Starch Adsorption Kinetics on Cellulose Fibers via the Modified Langmuir Adsorption Theory, Chemical and biochemical engineering quarterly, Volume: 23 Issue: 4 Pages: 461–470. Published: Dec. 2009.
- Šrekl, Jože, Golob, Janvit, Statistical Modeling in Fire-ignition Hazard Evaluation, Chemical and biochemical engineering quarterly, Volume: 23 Issue: 3 Pages: 309–315. Published: Sep. 2009.
- Zakrajšek, Nejc, Fuente, E., Blanco, A., Golob, Janvit, Influence of Cationic Starch Adsorption on Fiber Flocculation, Chemical engineering & technology, Volume: 32 Issue: 8 Pages: 1259–1265. Published: Aug. 2009.
- Zakrajšek, Nejc, Golob, Janvit, The Influence of Modified Starch on the Process Water Quality in Papermaking and the Paper Properties, Starch-Stärke, Volume: 61, Issue: 2 Pages: 109–115. Published: Feb. 2009.

### PRODUCT ENGINEERING RESEARCH FOR SUSTAINABLE DEVELOPMENT

*Publications:*

- Gregori, Andrej, Švagelj, Mirjan, Berovič, Marin, Liu, Y., Zhang, Jingsong, Pohleven, Franc, Klinar, Dušan, Cultivation and bioactivity assessment of Grifola frondosa fruiting bodies on olive oil press cakes substrates, New biotechnology, Volume: 26 Issue: 5 Pages: 260–262. Published: Nov. 2009.

## OTHER RELEVANT ACHIEVEMENTS

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

*Contributions at international meetings:*

- Šoštarič, Maja, Selišnik, Aljaž, Knez, Sergej, Golob, Janvit, Bricelj, Mihael, Klinar, Dušan, Pivec, Aleksandra. Studies on growth of *Chlorella vulgaris* under different cultivation conditions. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.

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

*Contributions at international meetings:*

- Zakrajšek, Nejc, Golob, Janvit, Knez, Sergej, Ravnjak, David. The influence of modified starch on the process water quality in the papermaking. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.
- Klofutar, Boštjan, Golob, Janvit, Klofutar, Cveto, Žagar, Ema, Poljanšek, Ida. Kinetics of the transesterification of rapeseed and waste sunflower oils. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.
- Šrekl, Jože, Golob, Janvit. New approach to calculate the probability of ignition : [lecture]. V: 8th World congress of chemical engineering incorporating the 58th Canadian chemical engineering conference and the XXIV Interamerican congress of chemical engineering : Montreal, Quebec, Canada, August 23–27, 2009 : WCCE8.

### PRODUCT ENGINEERING REASEARCH FOR SUSTAINABLE DEVELOPMENT

*Contributions at international meetings:*

- Likozar, Blaž, Modeling of elastomer cross-linking by organic peroxides : correlation of kinetics, mass transfer, heat transfer and viscoelasticity. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, p. 97.

- Likozar, Blaž, Kinetic modelling of the peroxide cross-linking of polymer/monomer blends : from a theoretical model framework to its application for a complex polymer/monomer system. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, p. 98.
- Likozar, Blaž, Major, Zoltan, The influence of nitrile content, hydrogenation and compound preparation on morphological, mechanical, thermal and other properties of (hydrogenated) nitrile rubber/carbon nanotube nanocomposites. V: European Polymer Congress [tudi] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, p. 151.
- Likozar, Blaž, Major, Zoltan, Modelling of the filled elastomer moduli of unfunctionalized, hydroxy-, and carboxy- functionalized multi-walled carbon nanotubes reinforced hydrogenated nitrile rubber and the morphology of nanocomposites. V: European Polymer Congress [also] EPF'09, Graz, Austria, 12.–17. 7. 2009. Book of abstracts and basic information about the congress. Graz: Graz University of Technology, Institute for Chemistry and Technology of Materials [etc.], 2009, p. 151.
- Likozar, Blaž, Major, Zoltan, Modelling of the filled elastomer moduli of unfunctionalized, hydroxy-, and carboxy- functionalized multi-walled carbon nanotubes reinforced hydrogenated nitrile rubber and the morphology of nanocomposites. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, p. 17.
- Likozar, Blaž, Major, Zoltan. The influence of nitrile content, hydrogenation and compound preparation on morphological, mechanical, thermal and other properties of (hydrogenated) nitrile rubber/carbon nanotube nanocomposites. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, p. 18.
- Likozar, Blaž, Kinetic modelling of the peroxide cross-linking of polymer/monomer blends : from a theoretical model framework to its application for a complex polymer/monomer system. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, p. 23.
- Likozar, Blaž, Modeling of elastomer cross-linking by organic peroxides : correlation of kinetics, mass transfer, heat transfer and viscoelasticity. V: Polymer Reaction Engineering VII, May 3–8, 2009, Niagara Falls, Ontario, Canada. Program. New York: Engineering Conferences International, 2009, p. 24.

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, ie. 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 knowledge will be transferred into industrial plants.

# 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 Stefan. Kot infrastrukturni center je namenjen za znanstveno-raziskovalno, razvojno in izobraževalno dejavnost. 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 drugih sodelavcev fakultete v sistem 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 2009

## CHAIRS IN 2009

# 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 Kebe

**Raziskovalci** / Researchers
izr. prof. dr. Matija Strlič (v dopolnilnem razmerju / *part-time*)
dr. Jana Kolar (v dopolnilnem razmerju / *part-time*)
Danijela Pucko, dipl. inž. kem. tehn.
dr. Martin Šala

**Tehniki** / Technicians
Zdenka Držaj
Jolanda Furlan
Mojca Žitko

| **Mladi raziskovalci**<br>*Young Researchers* | Mentor<br>*Mentor* | Čas usposabljanja<br>*Programme Duration* | Oblika usposabljanja<br>*Degree* |
|---|---|---|---|
| Tanja Trafela | M. Strlič | 2006–2010 | doktorski študij / *PhD* |
| Gregor Arh | M. Veber | 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

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

- Analitika in spektroskopija / *Chemical Analysis and Spectroscopy* – VS
- Analizna kemija / *Analytical Chemistry* – UN – Kemija / *Chemistry*
- Analizna kemija / *Analytical Chemistry* – UN – Kemijsko inženirstvo / *Chemical Engeneering*
- 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

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

- Analizna kemija in okolje / *Environmental Analytical Chemistry*
- Elektrokemijske analizne metode / *Electroanalytical Methods*
- Infrardeča in ramanska spektroskopija / *Infrared and Raman Spectroscopy*
- Izbrane metode analizne spektroskopije / *Selected Topics in Analytical Spectroscopy*
- Izbrane metode instrumentalne analize / *Selected Methods in Instrumental Analysis*
- Kemija in analiza naravnih vod / *Chemistry and Analysis of Natural Waters*
- Kovine v bioloških sistemih / *Metals in Biological Systems*
- Masna spektrometrija / *Mass Spectromety*
- Radiokemijske metode analize / *Radiochemical Methods of Analysis*
- Separacijske metode v kemijski analizi / *Separation Techniques in Analytical Chemistry*
- Uvod v metode umetne inteligence v kemiji / *Fundamentals of Artificial Intelligence Methods in Chemistry*

## IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1<sup>st</sup> 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*

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Analizna kemija / *Analytical Chemistry* PEF – UN

Kemija okolja / *Environmental Chemistry* PEF – UN

Bolonjski programi 3. stopnje / *Bologna 3<sup>rd</sup> 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*

Predbolonjski univerzitetni podiplomski študijski programi (UPŠ Varstvo okolja) / *Pre-Bologna Postgraduate University Study Programme in Environmental Protection*

Analizna kemija v kontroli okolja / *Analytical Chemistry in Environmental Control*

Kemijski procesi v okolju / *Chemical Processes in Environment*

## 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, characterization 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 / AWARDS, RECOGNITIONS

- M. Veber, Zlata plaketa Univerze v Ljubljani / *Golden Medal of the University of Ljubljana*

## 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*

Skupaj z NUK / *Sharing 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*

## **RAZISKOVALNI PROGRAMI IN PROJEKTI** / RESEARCH PROGRAMMES AND PROJECTS

### **RAZISKOVALNI PROGRAMI** / RESEARCH PROGRAMMES

| | |
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| P1–0153 | Raziskave in razvoj analiznih metod in postopkov / *Research and Development of Analytical Methods and Procedures*<br>Vodja programa / *Principal Researcher*: B. Pihlar |

### **APLIKATIVNI PROJEKTI** / APPLIED RESEARCH

| | |
|---|---|
| L1–9710 | PAPERVOC: Hlapne organske snovi v zbirkah kulturne dediščine na papirju – vir informacij ali zdravstveno tveganje? / *Volatile Organic Compounds in Paper-Based Cultural Heritage Collections – Source of Information or Health Risk?*<br>Nosilec / *Principal Researcher*: M. Strlič<br>Sofinancer / *Co-sponsored by:* Nationaal Archief, Haag, Nizozemska |
| L1–7165 | Transformacija onesnaževal z ozonom in naprednimi postopki oksidacije / *Transformation of Pollutants Using Ozone and Advanced Oxidation Procedures*<br>Nosilec / *Principal Researcher*: M. Strlič<br>Sofinancer / *Co-sponsored by:* Zavod za varstvo pri delu |

## 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)*<br>Nosilka / *Principal Researcher*: N. Gros |
| COST D42 | *Chemical Interactions between Cultural Artefacts and the Indoor Environment – EnviArt*<br>Nosilec / *Principal Researcher*: M. Strlič |
| Eureka 3483 | *Advanced Laser Renovation of Old Paintings, Paper, Parchment and Metal Objects*<br>Nosilec / *Principal Researcher*: M. Strlič |
| FOOD – CT – 2006 –016264 EU 6. OP | *Traditional Europe Food (TRUEFOOD)*<br>Nosilec / *Principal Researcher*: M. Pompe |
| CHRESP EU 7. OP | *"8th European Conference on Research for Protection, Conservation and Enhancement of Cultural Heritage"*<br>Nosilec / *Principal Researcher*: M. Strlič |

### BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

| | |
|---|---|
| Slovenija – Hrvaška<br>*Slovenia – Croatia* | Nastanek, transport in razgradnja fotooksidantov na področju Mediterana / *Formation, Transport and Degradation of Photooxidants in the Mediterranean*<br>Nosilec / *Principal Researcher*: M. Pompe |
| Slovenija – Kitajska<br>*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*<br>Nosilec / *Principal Researcher*: M. Pompe |
| Slovenija – ZDA<br>*Slovenia – USA* | Kvantitativna ocena tveganja pri tradicionalnih izdelkih živil / *Quantitative Risk Assessment of Traditional Food Products*<br>Nosilec / *Principal Researcher*: M. Veber |

| | |
|---|---|
| Slovenija – Romunija<br>*Slovenia – Romania* | Razvoj spektroskopskih metod za kontrolo kvalitete proteinskih materialov / *Development of Spectroscopic Methods for Quality Control of Proteinaceus Materials*<br>Nosilec / *Principal Researcher*: M. Strlič |
| Slovenija – Turčija<br>*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*<br>Nosilec / *Principal Researcher*: M. Pompe |

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*AL2.* 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.], str. 1–8. [COBISS.SI-ID 33467909]

*AL3.* KITAHARA, Yuki, TAKAHASHI, Seiji, KURAMOTO, Noriyuki, ŠALA, Martin, TSUGOSI, Takahisa, SABLIER, Michel, FUJII, Toshihiro. Ion attachment mass spectrometry combined with infrared image furnace for thermal analysis : evolved gas analysis studies. *Anal. chem. (Wash.)*. [Print ed.], 2009, vol. 81, no. 8, str. 3155–3158. [COBISS.SI-ID 30312965]

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*AL23.* VIDIC, Iztok, ZUPANČIČ-KRALJ, Lucija, SEPČIĆ, Kristina, POHLEVEN, Franc. Decay of polychlorinated biocides by wood rooting fungi : [invited lecture]. V: RADONJIĆ, Veselin B. (ur.). *Proceedings of 6th International symposium on biocides in public health and environmental protection [and] The 6th International symposium on antisepsis, disinfection and sterilization [and] Belgrade 2009 conference on vector control in urban environments, October 06–07. 2009, Belgrade, Serbia*. Belgrade: Institute for biocides and medical ecology, 2009, str. 68–75, graf. prikazi. [COBISS.SI-ID 1766281]

*AL24.* VRŠČAJ VODOŠEK, Tatjana, KRALJ CIGIĆ, Irena, STRLIČ, Matija, KOŠMERL, Tatjana. Evolution of aroma compounds during malolactic fermentation of cool-climate varieties Welsh Riesling and Sauvignon. V: The XXI-es Entretiens Scientifiques Lallemand and the 115th Anniversary of The Geisenheimer Hefe-Reinzucht-Station, Geisenheim, Germany, April 24, 2009. *Sensory development of cool-climate varietals during wine fermentation : proceedings*. Gesenheim: Geseinheim Institute, 2009, str. [1–10, sprejeto v tisk]. [COBISS.SI-ID 3636856]

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## **SAMOSTOJNI ZNANSTVENI SESTAVEK ALI POGLAVJE V MONOGRAFSKI PUBLIKACIJI** / INDEPENDENT SCIENTIFIC COMPONENT PART IN A MONOGRAPH

*AL31.* PAJAGIČ BREGAR, Gojka, VELUŠČEK, Anton, TOLAR, Tjaša, STRLIČ, Matija, BUKOŠEK, Vili, KOLAR, Jana, RAVBAR, Igor. Raziskave in konserviranje preje z Ljubljanskega barja = Analysis and conservation of the Ljubljansko barje yarn. V: VELUŠČEK, Anton (ur.). *Koliščarska naselbina Stare gmajne in njen čas : Ljubljansko barje v 2. polovici 4. tisočletja pr. Kr. : the Ljubljansko barje in the 2nd half of the 4th millennium BC*, (Opera Instituti archaeologici Sloveniae, 16). Ljubljana: Inštitut za arheologijo ZRC SAZU: Založba ZRC, 2009, str. 309–318, ilustr. [COBISS.SI-ID 30569773]

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## **UNIVERZITETNI ALI VISOKOŠOLSKI UČBENIK Z RECENZIJO** / REVIEWED UNIVERSITY AND ACADEMIC TEXTBOOK

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## **KONČNO POROČILO O REZULTATIH RAZISKAV** / FINAL RESEARCH REPORT

*AL35.* STRLIČ, Matija, TRAFELA, Tanja, CSEFALVAYOVA, Linda, KRALJ CIGIĆ, Irena, PIHLAR, Boris, KOLAR, Jana, BALAŽIC, Aneta, LICHTBLAU, Dirk Andreas, ANDERS, Manfred, BRUIN, G. de, KNIGHT, Barry, MARTIN, Graham, PALM, Jonas, SELMANI, Nikša, CHRISTENSEN, Mads Christian. *Final activity report : SSPI-006594 : SurveNIR : Near infrared spectroscopy tool for collection surveying*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, 2009. 62 str., ilustr. [COBISS.SI-ID 30430469]

## **UREDNIK** / EDITORSHIP

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# KATEDRA ZA ANORGANSKO KEMIJO
## CHAIR OF INORGANIC CHEMISTRY

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**prof. dr. Iztok Turel**

### SODELAVCI KATEDRE / PERSONNEL

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izr. prof. dr. Boris Čeh
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Petra Vuković
Igor Ponikvar
Vinko Volk

| **Mladi raziskovalci**<br>*Young Researchers* | Mentor<br>*Mentor* | Čas usposabljanja<br>*Programme Duration* | Oblika usposabljanja<br>*Degree* |
|---|---|---|---|
| Simona Medvešček | A. Meden | 2003–2010 | doktorski študij / *PhD* |
| Katarina Stare (Demšar) | A. Meden | 2006–2010 | 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* |

# 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*

Splošna kemija / *General Chemistry* – UN in VS
Praktikum iz splošne in anorganske kemije / *Practicals in General and Inorganic Chemistry* – UN
Anorganska kemija / *Inorganic Chemistry* – UN in VS
Zgradba in lastnosti trdnin / *Structure and Properties of Solids* – UN
Anorganska sinteza / *Inorganic Synthesis* – UN in VS
Kemija za trajnostni razvoj / *Chemistry for Sustainable Development* – UN
Kemijski praktikum / *Chemical Practicum* – UN

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Kemija in kemijska tehnologija / *Chemistry and Chemical Technology* – VS

- 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
- Kemija kompleksov / *Chemistry of Complexes* – UN
- Kristalna kemija / *Crystal Chemistry* – UN
- Metodika anorganskih eksperimentov / *Methodology of Inorganic Experiments* – UN
- Teorija gorenja, gašenja in dinamika procesov / *Theory of Combustion, Extinction and Fire Dynamics* – VS

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*
- Bioanorganska kemija / *Bioinorganic Chemistry*
- Kemija trdnega stanja / *Solid State Chemistry*
- Organokovinska kemija / *Metal-Organic Chemistry*
- Termična analiza / *Thermal Analysis*
- Kristalografija v biokemiji / *Crystallography in Biochemistry*

## IZVEN FKKT / EXTRAMURAL COURSES

Bolonjski programi 1. stopnje / *Bologna 1st Cycle Study Programmes*

- Kemija / *Chemistry* FS – UN
- Kemija / *Chemistry* NTF – UN in VS
- Kemija / *Chemistry* FMF – UN in VS
- Osnove kemije / *Fundamentals of Chemistry* FGG – UN
- Splošna kemija / *General Chemistry* BF – UN
- Anorganska kemija / *Inorganic Chemistry* FFA – UN
- Splošna in organska kemija / *General and* Organic *Chemistry* FFA – UN
- Anorganska kemija / *Inorganic Chemistry* NTF – UN
- Splošna in fizikalna kemija / *General and Physical Chemistry* BF – 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 the Type of Metal Ion Bonding in Wood*
- 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 such as Hialuronic Acid*
- Imobilizacija kovinskih zvrsti v kontaminirani zemlji / *Immobilization of Metal Species in Contaminated Soil*
- Imobilizacija kovinskih zvrsti v onesnaženih tleh in trdnih odpadkih / *Immobilization of Metal Species 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

### **NAGRADE, PRIZNANJA** / AWARDS, RECOGNITIONS

- I. Leban, Priznanje »Prometej znanosti za odličnost v komuniciranju« (Slovenska znanstvena fundacija) / *I. Leban, "Special Achievement for Excellency in Scientific Communication" (The Slovenian Science Foundation)*
- T. Birsa Čelič, Prešernova nagrada FKKT za leto 2009 (mentorica A. Golobič) / *The Faculty Prešeren Award for 2009*

## 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*
- A. Demšar, 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 18. slovensko-hrvaškega srečanja kristalografov (Varaždin, Hrvaška) / *Co-chairman of the Organising Committee of the 18th Slovenian-Croatian Crystallographic Meeting (Varaždin, Croatia)*

## DRUGO / OTHER

- I. Leban, ekspert v Institutional Evaluation Programme Evropskega združenja univerz (EUA) / *Expert in the Institutional Evaluation Programme, European Universities Association*
- I. Leban, »Noč raziskovalcev 2009«, eksperimentalno predavanje za popularizacijo kemije / *"Researchers' Night 2009" – Demonstration Lecture for the Popularization of Chemistry*
- S. Petriček, predsednica Državne predmetne komisije za splošno maturo iz kemije / *Chairman of the Subject Testing Committee for the Matura in Chemistry*

# 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 + Modul for Thermoluminescence with PRO. sensicam)*
- 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 Euraf CAD 4 / *Single-Crystal Diffractometer Nonius Euraf CAD 4*
- Difraktometer za monokristale Nonius Kappa CCD 4 + kriostat za tekoči dušik Oxford Cryosystem 700 / *Single-Crystal Diffractometer Nonius Kappa CCD 4 + Oxford Cryosystem 700 for Liquid Nitrogen*

- Visoko ločljivi rentgenski praškovni difraktometer s CuK$_{\alpha1}$ 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*

## RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

### RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

| | |
|---|---|
| P1–0134 | Bioanorganska in bioorganska kemija / *Bioinorganic and Bioorganic Chemistry*<br>Vodja programa / *Principal Researcher*: P. Bukovec |
| P1–0175 | Sinteza, struktura, lastnosti snovi in materialov / *Synthesis, Structure and Properties of Compounds and Materials*<br>Vodja programa / *Principal Researcher*: I. Leban |

### TEMELJNI PROJEKTI / BASIC RESEARCH

| | |
|---|---|
| J1–0200 | Sinteza novih protitumorskih rutenijevih spojin / *Synthesis of Novel Antitumor Ruthenium Compounds*<br>Nosilec / *Principal Researcher*: I. Turel |

### APLIKATIVNI PROJEKTI / APPLIED RESEARCH

| | |
|---|---|
| L2–1129 | Razvoj fotokatalitskih prevlek in plinskih fotoreaktorjev / *Development of Photocatalytic Coatings and Gas Photoreactors*<br>Nosilec / *Principal Researcher*: P. Bukovec<br>Sofinancer / *Co-sponsored by*: Martex d.o.o. |

| | |
|---|---|
| L4–2144 | Premazi iz utekočinjenega lesa / *Liquified Wood Coatings*<br>Nosilec / *Principal Researcher*: P. Bukovec<br>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)*
- Salonit d.d.: Kvantitativne fazne analize (letna pogodba) / *Quantitative Phase Analyses (Annual Contract)*

### RAZISKOVALNI PROJEKTI (DRUGI NAROČNIKI) / RESEARCH PROJECTS (OTHER CONTRACTORS)

| | |
|---|---|
| ESS – Evropski socialni sklad – projekti / *European Social Fund* | Partnerstvo fakultet in šol: vseživljenjsko učenje učiteljev naravoslovnih predmetov / *Partnership of Faculties and Schools: Life-Long Learning of Science Teachers*<br>Koordinator projekta: Fakulteta za kemijo in kemijsko tehnologijo / *Coordination of the Project: Faculty of Chemistry and Chemical Technology*<br>Vodja projekta / *Head of the Project*: N. Bukovec<br>Financer: Evropski socialni sklad ter Ministrstvo za šolstvo in šport RS / *Sponsored by: European Social Fund and the Ministry of Education and Sports of the Republic of Slovenia* |

## MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

### VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

| | |
|---|---|
| COST D39 | *Metallo-Drug Design and Action*<br>Nosilec / *Principal Researcher*: S. Grabner |
| COST 540 | *Photocatalytic Technologies and Novel Nanosurface Materials*<br>Članica upravnega odbora / *Steering Committe Member*: R. Cerc Korošec |
| COST D39 | *Ruthenium Anticancer Compounds*<br>Nosilec / *Principal Researcher*: I. Turel |

## BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

| | |
|---|---|
| Slovenija – Srbija<br>*Slovenia – Serbia* | Struktura in mikrostruktura oksidnih nanomaterialov / *Structure and Microstructure of Oxide Nanomaterials*<br>Nosilec / *Principal Researcher*: A. Meden |
| Slovenija – Avstrija<br>*Slovenia – Austria* | Rutenijeve spojine in njihova možna uporaba v elektrokemoterapiji / *Ruthenium Compounds and their Possible Applications in Electrochemotherapy*<br>Nosilec / *Principal Researcher*: I. Turel |

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## IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

*AK1.* PETRIČEK, Saša. Synthesis and structural similarities of yttrium and lanthanide chloride complexes with diglyme and tetrahydrofuran. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 2, str. 426–433. [COBISS.SI-ID 30530565]

*AK2.* FRLAN, Rok, PERDIH, Franc, CIRKVENČIČ, Nina, PEČAR, Slavko, OBREZA, Aleš. Design and synthesis of novel UDP-Mur-NAc, UDP-Mur-NAc-L-Ala and UDP-Mur-NAc-L-Ala-D-Glu mimetics. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 3, str. 580–590. [COBISS.SI-ID 30810885]

*AK3.* KASUNIČ, Marta, MEDEN, Anton, ŠKAPIN, Srečo D., SUVOROV, Danilo, GOLOBIČ, Amalija. Order-disorder of oxygen anions and vacancies in solid solutions of La[sub]2TiO[sub]5 and La[sub]4Ga[sub]2O[sub]9. *Acta crystallogr., B Struct. sci.*, 2009, vol. B65, no. 5, str. 558–566. [COBISS.SI-ID 30821637]

*AK4.* ČASAR, Zdenko, LEBAN, Ivan, MAJCEN LE MARECHAL, Alenka, PIEKARA-SADY, Lidia, LORCY, Dominique. Charge transfer complexes and cation radical salts of azino-diselenadiazafulvalene. *C. r., Chim.*, Sep. 2009, tome 12, fascicule 9, str. 1057–1065. [COBISS.SI-ID 13221398]

*AK5.* MOLČANOV, Krešimir, KOJIĆ-PRODIĆ, Biserka, MEDEN, Anton. Unique electronic and structural properties of 1,4-benzoquinones : crystallochemistry of alkali chloranilate hydrates. *Croat. chem. acta*, 2009, vol. 82, no. 2, str. 387–396. [COBISS.SI-ID 30847493]

*AK6.* KOZLEVČAR, Bojan, KOVŠCA, Igor, JAGLIČIĆ, Zvonko, PEVEC, Andrej, KITANOVSKI, Nives, STRAUCH, Peter, ŠEGEDIN, Primož. Strong antiferromagnetism in isolated anionic dicopper(II) methanoato paddle-wheel complex. *Croat. chem. acta*, 2009, vol. 82, no. 2, str. 463–467. [COBISS.SI-ID 30626053]

*AK7.* KITANOVSKI, Nives, GOLOBIČ, Amalija, ČEH, Boris. Two compounds with trans-[Mo(NCS)[sub]4([gamma]-pic)[sub]2][sup]- anion. *Croat. chem. acta*, 2009, vol. 82, no. 3, str. 567–571. [COBISS.SI-ID 30773765]

*AK8.* ZUPANČIČ JUSTIN, Maja, ZUPANČIČ, Marija. Combined purification and reuse of landfill leachate by constructed wetland and irrigation of grass and willows. *Desalination*. [Print ed.], 2009, vol. 246, no. 1/3, str. 157–168. [COBISS.SI-ID 30489093]

*AK9.* URŠIČ, Uroš, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. [2+2] Cycloadditions of electron-poor acetylenes to (5Z)-5-[(dimethylamino)methylene]imidazolidine-2,4-diones. *Helv. Chim. Acta*, 2009, vol. 92, no. 3, str. 481–490. [COBISS.SI-ID 30316805]

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*AK11.* TANG, Jinkui, COSTA, José Sánchez, GOLOBIČ, Amalija, KOZLEVČAR, Bojan, ROBERTAZZI, Arturo, VARGIU, Attilio V., GAMEZ, Patrick, REEDIJK, Jan. Magnetic coupling between copper(II) ions mediated by hydrogen-bonded (neutral) water molecules. *Inorg. chem.*, 2009, vol. 48, no. 12, str. 5473–5479. [COBISS.SI-ID 30579205]

*AK12.* BUKOVEC, Peter, KROŠELJ, Vesna, TURK, Samo, VREČER, Franc. Optimization of melt pelletization in a high shear mixer. *Int. j. pharm.* [Print ed.], 2009, no. 2, vol. 381, str. 192–198. [COBISS.SI-ID 2621553]

*AK13.* KRANJC, Krištof, PERDIH, Franc, KOČEVAR, Marijan. Effect of ring size on the exo/endo selectivity of a thermal double cycloaddition of fused pyran-2-ones. *J. org. chem.*, 2009, vol. 74, no. 16, str. 6303–6306. [COBISS.SI-ID 30678277]

*AK14.* KÜZMA, Mirjana, DOMINKO, Robert, MEDEN, Anton, MAKOVEC, Darko, BELE, Marjan, JAMNIK, Janko, GABERŠČEK, Miran. Electrochemical activity of Li[sub]2FeTiO[sub4 and Li[sub]2MnTiO[sub]4 as potential active materials for Li ion batteries: a comparison with Li[sub]2NiTiO[sub]4. *J. power sources*. [Print ed.], 2009, issue 1, vol. 189, str. 81–88. [COBISS.SI-ID 4119578]

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*AK16.* LOZINŠEK, Matic, BUNIČ, Tina, GORESHNIK, Evgeny A., MEDEN, Anton, TRAMŠEK, Melita, TAVČAR, Gašper, ŽEMVA, Boris. Syntheses, crystal structures and Raman spectra of Ba(BF[sub]4)(PF[sub]6), Ba(BF[sub]4)(AsF[sub]6)and Ba[sub]2(BF[sub]4)[sub]2(AsF[sub]6)(H[sub]3F[sub]4) : the first examples of metal salts containing simultaneously tetrahedral (BF[sub]4)[sup]- and octahedral (AF)[sub]6[sup]- anions. *J. solid state chem.*, 2009, vol. 182, no. 10, str. 1897–2903. [COBISS.SI-ID 22845991]

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*AK25.* MAVER, Ksenija, LAVRENČIČ ŠTANGAR, Urška, ČERNIGOJ, Urh, GROSS, Silvia, CERC KOROŠEC, Romana. Low-temperature synthesis and characterization of TiO [sub] 2 and TiO [sub] 2-ZrO [sub] 2 photocatalytically active thin films. *Photchem. photobiol. sci. (Print)*, 2009, vol. 8, no. 5, str. 657–662. [COBISS.SI-ID 1104123]

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## PREGLEDNI ZNANSTVENI ČLANEK / REVIEW ARTICLE

*AK33.* SEPČIĆ, Kristina, PERKOVIĆ, Olivio, TUREL, Iztok, SEPČIĆ, Juraj. Nuspojave i interakcije fluorokinolona = Adverse effects and interactions of fluoroquinolones. *Liječ. vjesn.*, 2009, letn. 131, št. 3–4, str. 74–80. [COBISS.SI-ID 25736665]

## OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

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# KATEDRA ZA BIOKEMIJO
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| **Mladi raziskovalki**<br>*Young Researchers* | Mentor<br>*Mentor* | Čas usposabljanja<br>*Programme Duration* | Oblika usposabljanja<br>*Degree* |
|---|---|---|---|
| Nataša Lindič | N. Lovšin | 2009–2013 | doktorski študij / *PhD* |
| Nives Škrlj | M. Dolinar | 2006–2011 | 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*

- Molekularne osnove ved o življenju / *Molecular Fundamentals of Life Sciences* – UN
- Temelji biokemije / *Biochemistry Fundamentals* – UN
- Biokemijski praktikum / *Biochemistry Practicals* – UN

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

- Biokemija / *Biochemistry* – UN
- Biokemijska informatika / *Bioinformatics* – UN
- Encimatika / *Enzymology* – UN
- Tehnologija rekombinantne DNA / *Recombinant DNA Technology* – UN
- Molekularna imunologija / *Molecular Immunology* – UN
- Metode določanja 3D strukture makromolekul / *Methods of 3D Structure Determination of Macromolecules* – 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*

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

- Biološke makromolekule / *Biological Macromolecules*

### IZVEN FKKT / EXTRAMURAL COURSES

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

- Biokemija / *Biochemistry* FFA – UN – Farmacija / *Pharmacy*
- Biokemija / *Biochemistry* FFA – VS – Laboratorijska biomedicina / *Laboratory Biomedicine*

Predbolonjski univerzitetni podiplomski študijski programi (UPŠ Biomedicina) / *Pre-Bologna Postgraduate University Study Programme in Biomedicine*

- Izbrani procesi iz biokemije in molekularne biologije / *Selected Topics in Biochemistry and Molecular Biology*
- Načela in tehnike v biokemiji in molekularni biologiji / *Principles and Methods in Biochemistry and Molecular Biology*
- Genetika / *Genetics*
- Jedrska magnetna resonanca za raziskave bioloških makromolekul / *Nuclear Magnetic Resonance for Investigations of Biological Macromolecules*
- Molekularna bioinformatika / *Molecular Bioinformatics*
- Eksperimentalne metode v raziskavah naravne imunosti / *Experimental Methods in Natural Immunity Research*
- Monoklonska protitelesa – pregled področja in možnosti njihove uporabe v raziskavah, diagnostiki in terapiji / *Monoclonal Antibodies – Review and Their Application forResearch, Diagnostics and Therapy.*
- Metode v eksperimentalni onkologiji / *Methods in Experimental Oncology*

## 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 in dinamiko transpozicijskih elementov. Drugi analizirajo toksične fosfolipaze (amoditoksine) pri modrasu in s pomočjo mutageneze ugotavljajo, kateri deli molekule so odgovorni za encimsko in nevrotoksično delovanje ter kako se vežejo na specifične vezavne proteine.

Sodelavci, ki so vključeni v programa Proteoliza in njena regulacija ter Strukturna biologija, analizirajo proteinaze in njihove inhibitorje, tako naravnega izvora kot tiste, ki jih pridobijo s tehnikami rekombinantne DNA. Izolaciji sledi študij lastnosti, predvsem interakcije proteinaz z inhibitorji in substrati, ugotavljanje odnosov med zgradbo in funkcijo ter določanje vloge, ki jih te molekule imajo v zdravi ali oboleli celici.

V sodelovanju z Zavodom za transfuzijsko medicino (skupina prof. dr. Vladke Čurin Šerbec) poteka priprava humaniziranih protiteles proti patogeni obliki priona. Takih protiteles človeški imunski sistem ne bi prepoznal in bi jih bilo mogoče uporabiti za zdravljenje. Humanizacija poteka po načelu prilagoditve površine mišjih protiteles. Aminokislinske ostanke, ki so značilni za mišje imunoglobuline, smo zamenjali s tistimi, ki jih najdemo pri človeških, nato pa smo v bakterijskih celicah izrazili enoverižne fragmente mišjega in humaniziranih protiteles.

Raziskave na temo človeške transmembranske epitelijske celične adhezijske molekule Ep-CAM, ki je (potencialna) tarča antitumorskih terapij, smo nadaljevali v okviru novega temeljnega raziskovalnega projekta. Gre za raziskave s strukturnega vidika, v okviru katerega smo že pripravili kvalitetne proteinske kristale za namen določitve strukture z rentgensko difrakcijo, ter s funkcijskega vidika v smislu interakcij z drugimi znotrajceličnimi in zunajceličnimi proteini. Tudi v tem delu projekta smo že prišli do prvih rezultatov, ki pa zahtevajo še nadaljnje raziskave.

Na osnovi sinteznobiološkega klonirnega vektorja pSB1 smo pripravili vektor pSB1K0prom za določanje moči promotorjev. Razviti sistem za vrednotenje promotorjev temelji na intenziteti transkripcije gena za aminoglikozid-fosfotransferazo, tako da je mogoče na osnovi antibiotičnega učinka kanamicina sklepati na raven izražanja tarčnega proteina. Hkrati smo razvili spletno aplikacijo PromCal, ki na osnovi dobljenih meritev gostote bakterijske kulture omogoči preračun kinetičnih parametrov in določitev relativne moči promotorja.

Človeški protein APOBEC3G preprečuje replikacijo številnim retrovirusom, tudi virusu HIV. Vpliv APOBEC3 na virusno okužbo smo preučevali pri miših. Virus M-MuLV povzroči bistveno hitrejšo in hujšo infekcijo pri miših brez APOBEC3, zato je pri miših z izključenim genom za APOBEC3 prišlo do razvoja levkemije bistveno počasneje kot pri miših divjega tipa.

Proteini APOBEC delujejo proti različnim retrovirusom, pa tudi retrotranspozonom. Preverjali smo, ali obstaja povezava med inhibitornim delovanjem proteinov APOBEC in sposobnostjo vezave retrotranspozonskega proteina pORF1 dolgega razpršenega elementa LINE-1 pri človeku. Čeprav je APOBEC3A najučinkovitejši preprečevalec retrotranspozicije LINE-1, nismo našli interakcij s proteinom pORF1. Zato predvidevamo, da proteini APOBEC3 preprečujejo retrotranspozicijo neodvisno od vezave na ta protein.

*The Chair is engaged in five research projects running within three different research programmes of the Jožef Stefan Institute: Toxins and Biomembranes, Proteolysis and its Regulation, and Structural Biology.*

*The research on toxinology focuses on the evolution and dynamics of transposition elements and on ammodytoxins (toxic phospholipases of the long-nosed viper). By site-directed mutagenesis it was possible to elucidate which regions of the molecule are involved in enzymatic and neurotoxic activity and the mode of binding to the specific binding proteins.*

*Those working on the Proteolysis and Structural Biology programmes are analyzing proteinases and their inhibitors of natural origin as well as those obtained by recombinant DNA techniques. Protein isolation is followed by characterization studies, mainly on protease interactions with target inhibitors and substrates, structure-function investigations, and determinations of the role in healthy and diseased human cells.*

*In cooperation with the National Blood Transfusion Center (the group of Prof. Vladka Čurin Šerbec) we are preparing humanized antibodies against the pathogenic form of the prion protein. Such antibodies would be shielded from the human immune system and could thus be used for therapy. Humanization is performed by resurfacing murine antibodies. We replaced potentially immunogenic sites on the surface of the murine immunoglobulin with human counterparts. In addition, we expressed single-chain antibody fragments of the murine and humanized antibodies in bacterial cells.*

*The research on human transmembrane epithelial cell adhesion molecule EpCAM, which is a potential target of antitumor therapies, was continued as a new basic research project. The work includes structural studies. We have already prepared quality crystals to determine the* *structure by using X-ray diffraction, as well as functional studies (interactions with other intracellular and extracellular proteins). Preliminary results have been obtained and we are currently analyzing them in detail.*

*On the basis of the synthetic biology cloning vector pSB1 we prepared pSB1J0prom, a specialized vector for promoter strength evaluation. The measurement system is based on the intensity of transcription of the aminoglycoside 3'-phosphotransferase gene (kanamycin resistance gene). Antibiotic resistance levels are reflected in different growth kinetics which is thus a relative measure of promoter strength. In parallel, we developed a Web-based application PromCal for the evaluation of experimental data.*

*Human APOBEC3G (hA3G) is a restriction factor for human immunodeficiency virus (HIV). The role of murine homologue (mA3) in restriction of retroviral infection was studied on mA3 –/– knockout mice. The mA3 +/+ mice infected by M-MuLV developed leukemia more slowly compared to the animals lacking one or both copies of mA3, indicating that mA3 restricts replication and pathogenesis of M-MuLV in vivo.*

*Members of the APOBEC family of enzymes exhibit inhibitory activity against a variety of retroviruses and retrotransposons. We examined whether the inhibitory effect of APOBEC3 proteins correlates with APOBEC3 ability to bind the LINE-1 ORF1 protein. Although human APOBEC3A shows the highest inhibitory potency against LINE-1 retrotransposon, no direct interactions were identified. We concluded that APOBEC3 proteins indirectly interfere with the LINE-1 retrotransposition pathway.*

## POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

### NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- R. Jerala je dobil Zoisovo nagrado za vrhunske dosežke na področju molekularne biologije in biotehnologije. Pomembne so predvsem njegove raziskave molekulskih mehanizmov obrambe pred virusnimi in bakterijskimi okužbami. Odkril je tudi nov način molekulskega prepoznavanja patogenov s pomočjo imunskega sistema, kar predstavlja pomemben prispevek k razumevanju imunske obrambe, razvoju novih protivirusnih učinkovin in tudi iskanju novih načinov zdravljenja avtoimunskih bolezni. */ R. Jerala was the recipient of the Zois Award for outstanding achievements in the field of molecular biology and biotechnology, namely in his investigations on the molecular defence mechanisms against viral and bacterial infections. He also discovered a new mode of molecular pathogen recognition by the immune system. This represents an important contribution towards understanding immune defence, development of new antiviral drugs and finding new ways of treatment of autoimmune diseases.*
- M. Dolinar in R. Jerala sta prejela Nagrado Maksa Samca za popularizacijo študijev UL FKKT predvsem za njuno vodenje izjemno uspešnih študentskih raziskovalnih ekip na tekmovanjih iz sintezne biologije iGEM. */ M. Dolinar and R. Jerala were awarded the Maks Samec Award for Popularization of Studies at the UL FKKT, most notably for their supervising of very successful student research teams in synthetic biology (iGEM competitions).*

- Univerzitetno Prešernovo nagrado za leto 2009 je dobil Peter Cimermančič, študent biokemije, za raziskovalno delo s področja bioinformatike. Delo z naslovom Identifikacija potencialnih tarč zdravilnih učinkovin v procesu jedrnega prenosa virusa HIV je pripravil od mentorstvu B. Lenarčič in somentorstvu A. Šalija. / *Peter Cimermančič, a biochemistry student, received the University Prešeren Award in 2009 for his research in bioinformatics (»Identification of potential drug targets in the process of the HIV nuclear transfer«) under the mentorship of B. Lenarčič (co-mentor A. Šali).*
- A. Ljubetič, Prešernova nagrada FKKT za leto 2009 (mentor R. Jerala) / *The Faculty Prešeren Award for 2009*
- A. Ondračka, Prešernova nagrada FKKT za leto 2009 (mentor R. Jerala) / *The Faculty Prešeren Award for 2009*
- M. Vizovišek, Prešernova nagrada FKKT za leto 2009 (mentor B. Turk) / *The Faculty Prešeren Award for 2009*
- D. Zafred, Prešernova nagrada FKKT za leto 2009 (mentor D. Turk) / *The Faculty Prešeren Award for 2009*
- U. Zelenko, Prešernova nagrada FKKT za leto 2009 (mentor R. Jerala) / *The Faculty Prešeren Award for 2009*

## **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*
- Čitalec mikrotitrskih ploščic Tecan Sunrise / *Microtiter Plate Reader Tecan Sunrise*
- Aparaturi za PCR Applied Biosystems GeneAmp 2700 in Veriti / *PCR Apparatuses Applied Biosystems GeneAmp 2700 and Veriti*
- Spektrofotometer za majhne volumne vzorcev Thermo Scientific NanoDrop 2000c / *Spectrophotometer for Small Sample Volumes Thermo Scientific NanoDrop 2000c*
- Ultrazvočni homogenizer Sartorius Labsonic M / *Ultrasound homogenizer Sartorius Labsonic M*
- Naprave za elektroforezno analizo proteinov in Western prenos / *Instruments for Electrophoretic Separations of Proteins and Western Blotting*
- Naprave za agarozno gelsko elektroforezo DNA / *Instruments for Agar Gel Electrophoresis DNA*
- Transiluminator / *Transilluminator*
- Sistem za dokumentacijo elektroforeznih gelov / *Electrophoresis Documentation System*
- Suhi inkubator in stresalnik za mikrobiologijo / *Incubators/Shakers*

- $CO_2$ inkubator / *$CO_2$ Incubator*
- Hlajeni inkubator / *Cooled Incubator*
- Frakcijski kolektor / *Fraction Collector*
- Mešalniki in vibracijski stresalniki / *Mixers and Shakers*
- Analitske tehtnice / *Analytical Balances*
- Čiste komore / *Clean Chambers*
- pH meter Mettler-Toledo / *pH Meter Mettler-Toledo*
- FPLC tekočinska kromatografija za hitro ločevanje proteinov / *Fast Protein Liquid Chromatograpy (FPLC)*
- HPLC tekočinska kromatografija visoke ločljivosti / *High Performance Liquid Chromatography (HPLC)*
- Vac koncentrator / *Vac Concentrator*
- Avtoklav / *Autoclave*
- Zmrzovalnik –80 ºC / *Freezer –80 ºC*
- Stereo mikroskop M7.5 Leica / *Stereo Microscope M7.5 Leica*
- Invertni mikroskop CKX-41 Olympus / *Inverted Microscope CKX-41 Olympus*

## **RAZISKOVALNI PROGRAMI IN PROJEKTI** / RESEARCH PROGRAMMES AND PROJECTS

### **RAZISKOVALNI PROGRAMI** / RESEARCH PROGRAMMES

| | |
|---|---|
| P1–0207 | Toksini in biomembrane / *Toxins and Biomembranes*<br>Vodja programa / *Principal Researcher*: I. Križaj (IJS) |
| P1–0140 | Proteoliza in njena regulacija / *Proteolysis and its Regulation*<br>Vodja programa / *Principal Researcher*: B. Turk (IJS) |
| P1–0048 | Strukturna biologija / *Structural Biology*<br>Vodja programa / *Principal Researcher*: D. Turk (IJS) |

### **RAZISKOVALNI PROJEKTI** / RESEARCH PROJECTS

| | |
|---|---|
| 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*<br>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*<br>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*<br>Nosilec / *Principal Researcher*: D. Kordiš |
| L3–0206 | Prioni v humani medicini: od strukturnih študij do aplikacij / *Prions in Human Medicine: From Structural Studies to Applications*<br>Nosilka / *Principal Researcher*: V. Čurin Šerbec |
| 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*<br>Nosilka / *Principal Researcher*: T. Lah Turnšek |

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# KATEDRA ZA FIZIKALNO KEMIJO
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|---|---|---|---|
| Mario Šimić | J. Lah | 2005–2009 | doktorski študij / *PhD* |
| 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* |

## IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

### IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

### FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

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
- Računalništvo in informatika / *Computer Science and Mathematics* – VS
- 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 3. stopnje / *Bologna 3$^{rd}$ 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 1$^{st}$ 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 / *Technology of Food Processing* BF – UN

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

- Fizikalna kemija / *Physical Chemistry* FFA – UN in VS
- 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 2$^{nd}$ Cycle Master Study Programmes*

- Fizikalna kemija / *Physical Chemistry* NTF – UN
- Fizikalna kemija polimerov / *Physical Chemistry of Polymers* NTF – UN

Bolonjski programi 3. stopnje / *Bologna 3$^{rd}$ 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

- M. Bončina, nagrada za najboljši poster na ICSC konferenci / *Best Poster Award at the ICSC Conference*
- V. Vlachy, izvolitev za rednega člana Evropske akademije znanosti in umetnosti / *Elected to the European Academy of Sciences and Arts (Academia Scientiarum et Artium Europaea)*
- V. Vlachy, član znanstvenega odbora konferenc z naslovom *»International Conference on Solution Chemistry«* (2003–2009)
- J. Koller, priznanje najboljšega predavatelja na študijskem programu Kemija v študijskem letu 2008/2009 po izboru študentov / *Students' Award as the Best Lecturer on Chemistry Study Programme in the School Year 2008/2009*

## 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,* 2004–
- M. Bešter Rogač, gostujoča urednica / *Guest Editor, Acta Chimica Slovenica*, 2009, 56 (1)
- G. Vesnaver, član uredniškega odbora / *Editorial Board Member, Acta Chimica Slovenica*, 1998–

## DRUGO / OTHER

- J. Dolenc, podoktorska štipendija na Zvezni tehniški visoki šoli (ETH), Zürich / *Post Doctoral Fellowship at ETH, Zürich*
- K. Kogej, štipendija Finske akademije za enomesečno bivanje na Univerzi v Helsinkih, Laboratorij za polimerno kemijo / *Scholarship of the Academy of Finland for a 30 Days Visit Stay at the University of Helsinki, Laboratory for Polymer Chemistry*

# 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 8 dvojedrnih 64 bitnih AMD Athlonov 64 X2 4200 / *Eight- Node Computer Cluster Based on Dual-Core AMD Athlon 64 X2 4200+ Server CPUs*

- 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, thermostat Lauda UB 40 (+/– 0,003 C), LCR Agilent 4284A, DMM Agilent 3458A z uporovnim termometrom Pt100, set različnih celic) / *System for High-Perfomance 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*<br>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*<br>Nosilka / *Principal Researcher*: J. Dolenc |

## RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

| | |
|---|---|
| BIO 05/2007 | Biofizikalno-kemijska karakterizacija rekombinantnih zdravil / *Biophysicochemical Characterisation of Recombinant Drugs*<br>Nosilca / *Principal Researchers*: J. Lah, G. Vesnaver<br>Financer / *Sponsored by:* Lek d.d. |
| BIO 05/2009 | Postavljanje platforme za fizikalno-kemijsko karakterizacijo proteinskih učinkovin / *Setting up the Platform for Physico-Chemical Characterization of Protein Substances*<br>Nosilec / *Principal Researcher*: J. Lah<br>Financer / *Sponsored by:* Lek d.d. |
| Pogodba št. I/8-106259/2008 | Študij in analiza farmacevtskih materialov / *Studies and Analysis of Pharmaceutical Materials*<br>Nosilec / *Principal Researcher*: J. Koller<br>Financer / *Sponsored by*: Krka d.d. |

## MEDNARODNO SODELOVANJE NA PODROČJU IZOBRAŽEVANJA / INTERNATIONAL COOPERATION IN THE FIELD OF EDUCATION

- A. Godec, mentor slovenske srednješolske ekipe na mednarodni kemijski olimpijadi v Cambridgeu, 2009 / *Mentor of the Slovenian Team at the International Chemistry Olympiad, Cambridge, 2009*
- 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. G. van Gunsteren)*
- Č. Podlipnik, gostujoči raziskovalec na Univerzi v Milanu, 1. junij–31. oktober, 2009 / *Visiting Researcher at the University of Milano, 1. June–31. October 2009*
- Podiplomski študent Erik Gutierrez Valladares, Universidad Nacional Autónoma de México, Mehika, september–december 2009, delovna mentorja: V. Vlachy in B. Hribar Lee / *Visiting Postgraduate Student*

## MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL SCIENTIFIC COOPERATION

### VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

| | |
|---|---|
| COST D31 | *Organising Noncovalent Chemical Systems with Selected Functions*<br>Nosilec / *Principal Researcher*: G. Vesnaver |
| COST D43 | *Colloid and Interface Chemistry for Nanotechnology*<br>Nosilka / *Principal Researcher:* M. Bešter Rogač |
| COST MP0802 | *Self-Assembled Guanosine Structures for Molecular Electronic Devices*<br>Koordinator / *Coordinator:* J. Lah |

## BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

| | |
|---|---|
| Slovenija – Avstrija<br>*Slovenia – Austria* | Kontrolirano sproščanje funkcionalnih molekul iz nosilnih sistemov iz novih materialov / *Controlled Release of Functional Molecules from Carrier Systems Made from New Materials*<br>Nosilec / *Principal Researcher:* M. Tomšič |
| Slovenija – Madžarska<br>*Slovenia – Hungary* | Obravnava strukture kompleksnih tekočin z metodama ozkokotnega rentgenskega sipanja in reverzne simulacije Monte Carlo / *Understanding the Structure of Complex Liquids by Small Angle Scattering and Reverse Monte Carlo Simulation*<br>Nosilec / *Principal Researcher:* A. Jamnik |
| Slovenija – ZDA (NIH)<br>*Slovenia – USA (NIH Grant)* | Solvatacija v bioloških sistemih/ *Solvation in Biology*<br>Nosilca / *Principal Researchers*: V. Vlachy, K. A. Dill (UC San Francisco) |
| Slovenija – Portugalska<br>*Slovenia – Portugal* | Vpliv hidrofobnosti in togosti polimerne verige na interakcije med polielektroliti in surfaktanti / *Effect of the Polymer Hydrophobicity and Backbone Rigidity on Polyelectrolyte-Surfactant Interactions*<br>Nosilka / *Principal Researcher*: K. Kogej |
| Slovenija – Finska<br>*Slovenia – Finland* | Asociacijski pojavi v vodnih raztopinah polielektrolitov ter polielektrolitov in surfaktantov / *Association Phenomena in Aqueous Polyelectrolyte and Polyelectrolyte/Surfactant Solutions*<br>Nosilka / *Principal Researcher*: K. Kogej |
| Slovenija – ZDA<br>*Slovenia – USA* | Modeli vode ter hidratacija preprostih in sestavljenih topljencev / *Models of Water and Hydration of Simple and Complex Solutes*<br>Nosilec / *Principal Researcher*: V. Vlachy |

## DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

### VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

- M. Bešter-Rogač*, Die Leitfähigkeit der Elektrolytlösungen-eine (nicht) beendete Geschichte,* Universität Regensburg, Institut für Physikalische und Theoretische Chemie, Regensburg, Germany, March 2009
- M. Bešter Rogač, *Electrolyte Solutions – a Challenge or Old News?,* Université Pierre et Marie Curie, Paris, France, June 2009
- K. Kogej, *Thermodynamics of the Conformational Transition of Atactic and Isotactic Polymethacrylic Acid in Aqueous Solution*, University of Helsinki, Helsinki, Finland, September 2009
- M. Lukšič, *From Electrolytes to Polyelectrolytes : Quenched-Annealed Systems and Ionenes,* Department of Chemical Engineering, The University of Texas at Austin, Austin, USA, August 2009
- V. Vlachy and M. Druchok, *Computer Simulations of Ionenes, Hydrophobic Ions with Unusual Solution Thermodynamic Properties*, UCSF Asilomar Meeting, Asilomar, California, USA, February 2009
- Yu. V. Kalyuzhnyi and V. Vlachy, *Aqueous Alkali Halide Solutions: Can Osmotic Coefficients be Explained on the Basis of the Ionic Sizes Alone*? UCSF Asilomar Meeting, Asilomar, California, USA, February 2009

- J. Dolenc, *GCN4 Coiled-Coil Trigger Sequence: Molecular Dynamics Simulation Techniques Resolve Apparent Inconsistencies Within Measured NMR Data,* Paul Scherrer Institute (PSI), Laboratory of Physical Chemistry, ETH Zürich, Zürich, Switzerland, May 2009
- J. Dolenc, *Thermodynamics of Sequence-Dependent Stability of DNA-Netropsin Complexes,* Vrije Universiteit, Amsterdam, The Netherlands, June 2009

### VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

- Prof. Dr. Nico van der Vegt, Center of Smart Interfaces, Technical University of Darmstadt, Germany, *Cationic Specific Binding with Protein Surface Charges,* June 2009
- Prof. Heikki Tenhu, University of Helsinki, Finland, *Functional Polymers and Hybrid Materials via Controlled Radical Polymerization*, October 2009
- Dr. Vladimir Asseyev, University of Helsinki, Finland, *Light Scattering in Polymer Chemistry,* April 2009

## BIBLIOGRAFIJA 2009 / REFERENCES 2009

### IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

*FK1.* BEŠTER-ROGAČ, Marija. Nonsteroidal anti-inflammatory drugs ion mobility : a condumetric study of salicylate, naproxen, diclofenac and ibuprofen dilute aqueous solutions. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 70–77. [COBISS.SI-ID 30281477]

*FK2.* PIÑERO, Jesus, BHUIYAN, Lutful B., REŠČIČ, Jurij, VLACHY, Vojko. Simulation of polyelectrolyte-catalysed reaction between divalent ions. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 115–123. [COBISS.SI-ID 30281733]

*FK3.* ZVONAR, Alenka, ROZMAN, Branka, BEŠTER-ROGAČ, Marija, GAŠPERLIN, Mirjana. The influence of microstructure on celecoxib release from a pharmaceutically applicable system: Mygliol 812/Labrasol/Plurol oleiquer/water mixtures. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 131–138. [COBISS.SI-ID 2523761]

*FK4.* ŠIMIĆ, Mario, VESNAVER, Gorazd, LAH, Jurij. Thermodynamic stability of the dimeric toxin CcdB. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 139–144. [COBISS.SI-ID 30281989]

*FK5.* LAJOVIC, Andrej, TOMŠIČ, Matija, JAMNIK, Andrej. Ordering of attractive colloids near a planar wall : theory and simulation. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 145–155. [COBISS.SI-ID 30282245]

*FK6.* PODLIPNIK, Črtomir. Docking of selected natural polyphenols to ARF activated A1 subunit of cholera toxin. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 156–165. [COBISS.SI-ID 30282501]

*FK7.* BIZJAK, Alan, URBIČ, Tomaž, VLACHY, Vojko. Phase diagram of the Lennard-Jones system of particles from the cell model and thermodynamic perturbation theory. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 166–171. [COBISS.SI-ID 30283013]

*FK8.* MARUŠIČ, Jaka, REŠČIČ, Jurij, JAMNIK, Andrej, TOMŠIČ, Matija. Salt-specific effects in solutions of human serum albumin : small-angle x-ray scattering and osmometry. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 172–179. [COBISS.SI-ID 30285829]

*FK9.* KLOFUTAR, Cveto, HORVAT, Jaka, BEŠTER-ROGAČ, Marija, RUDAN TASIČ, Darja. Viscosity of aqueous solutions of tetramethyl-, tetraethyl-, tetra-n-propyl-, tetra-n-butyl-, and tetra-n-pentylammonium cyclohexylsulfamates from 293.15 K to 323.15 K. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 188–195. [COBISS.SI-ID 30286085]

*FK10.* HRIBAR, Barbara, VLACHY, Vojko, DILL, Ken A. Modeling Hofmeister effects. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 1, str. 196–202. [COBISS.SI-ID 30286597]

*FK11.* PETERLIN, Primož, ARRIGLER, Vesna, KOGEJ, Ksenija, SVETINA, Saša, WALDE, Peter. Growth and shape transformations of giant phospholipid vesicles upon interaction with an aqueous oleic acid suspension. *Chem. phys. lipids*. [Print ed.], 2009, letn. 159, str. 67–76. [COBISS.SI-ID 25598681]

*FK12.* ŠIMIĆ, Mario, DE JONGE, Natalie, LORIS, Remy, VESNAVER, Gorazd, LAH, Jurij. Driving forces of gyrase recognition by the addiction toxin CcdB. *J Biol Chem*, 2009, vol. 284, no. 30, str. 20002–20010. [COBISS.SI-ID 30725381]

*FK13.* 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*, str. 1-5. [COBISS.SI-ID 33313541]

*FK14.* LAJOVIC, Andrej, TOMŠIČ, Matija, JAMNIK, Andrej. Depletion effects in a mixture of hard and attractive colloids. *J. chem. phys.*, 2009, vol. 130, no. 10, art. no. 104101 (10 str.).[COBISS.SI-ID 30270469]

*FK15.* DRUCHOK, M., VLACHY, Vojko, DILL, Ken A. Explicit-water molecular dynamics study of a short-chain 3,3 ionene in solutions with sodium halides. *J. chem. phys.*, 2009, vol. 130, no. 13, art. no. 134903 (8 str.). [COBISS.SI-ID 30353925]

*FK16.* JAMNIK, Andrej. Effective interaction between large colloidal particles immersed in a bidisperse suspension of short-ranged attractive colloids. *J. chem. phys.*, 2009, vol. 131, no. 16, art. no. 164111-1-1644111-8. [COBISS.SI-ID 33367045]

*FK17.* BIZJAK, Alan, URBIČ, Tomaž, VLACHY, Vojko, DILL, Ken A. Theory for the three-dimensional Mercedes-Benz model of water. *J. chem. phys.*, 2009, vol. 131, no. 19, art. no. 194504 (7 str.). [COBISS.SI-ID 33405957]

*FK18.* GUILLOT, S., TOMŠIČ, Matija, SAGALOWICZ, L., LESER, Martin E., GLATTER, Otto. Internally self-assembled particles entrapped in thermoreversible hydrogels. *J. colloid interface sci.*, 2009, vol. 330, no. 1, str. 175–179. [COBISS.SI-ID 30204933]

*FK19.* ŠARAC, Bojan, BEŠTER-ROGAČ, Marija. Temperature and salt-induced micellization of dodecyltrimethylammonium chloride in aqueous solution : a thermodynamic study. *J. colloid interface sci.*, 2009, vol. 338, no. 1, str. 216–221. [COBISS.SI-ID 30682117].

*FK20.* VALANT, Janez, DROBNE, Damjana, SEPČIĆ, Kristina, JEMEC, Anita, KOGEJ, Ksenija, KOSTANJŠEK, Rok. Hazardous potential of manufactured nanoparticles identified by in vivo assay. *J. hazard. mater.* [Print ed.], 2009, issues 1-3, vol. 171, str. 160–165, ilustr. [COBISS.SI-ID 6013049]

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*FK22.* CERKOVNIK, Janez, PLESNIČAR, Božo, KOLLER, Jože, TUTTLE, Tell. Hydrotrioxides rather than cyclic tetraoxides (tetraoxolanes) as the primary reaction intermediates in the low-temperature ozonation of aldehydes. The case of benzaldehyde. *J. org. chem.*, 2009, vol. 74, no. 1, str. 96–101. [COBISS.SI-ID 30098181]

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## KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

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## OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

*FK38.* LAJOVIC, Andrej, TOMŠIČ, Matija, JAMNIK, Andrej. Struktura tekočih primarnih alkoholov in aldehidov = Structure of liquid primary alcohols and aldehydes. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2009, Maribor, 24. in 25. september 2009*. Maribor: FKKT, [2009], str. [1–8]. [COBISS.SI-ID 30840581]

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## SAMOSTOJNI ZNANSTVENI SESTAVEK ALI POGLAVJE V MONOGRAFSKI PUBLIKACIJI / INDEPENDENT SCIENTIFIC COMPONENT PART IN A MONOGRAPH

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## SREDNJEŠOLSKI, OSNOVNOŠOLSKI ALI DRUGI UČBENIK Z RECENZIJO / REVIEWED SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK

*FK42.* GODEC, Andrej, LEBAN, Ivan. *Atomi in molekule, Učbenik za kemijo v gimnaziji*. 1. izd. Ljubljana: Modrijan, 2009. 159 str., ilustr. ISBN 978-961-241-323-1. [COBISS.SI-ID 244693248]

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## DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

*FK45.* BONČINA, Matjaž, CERAR, Janez, LAJOVIC, Andrej, LUKŠIČ, Miha, PRISLAN, Iztok. *Laboratorijske vaje iz fizikalne kemije za študente laboratorijske biomedicine : študijsko leto 2009/2010 : (interno gradivo)*. Ljubljana: Univ. v Ljubljani, Fak. za kemijo in kemijsko tehnologijo, Katedra za fizikalno kemijo, 2009. 47 str., graf. prikazi. [COBISS.SI-ID 33289733]

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## **PREDAVANJE NA TUJI UNIVERZI** / INVITED LECTURE AT A FOREIGN UNIVERSITY

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## **UREDNIK** / EDITORSHIP

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# KATEDRA ZA ORGANSKO KEMIJO
## CHAIR OF ORGANIC CHEMISTRY

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| **Mladi raziskovalci**<br>*Young Researchers* | Mentor<br>*Mentor* | Čas usposabljanja<br>*Programme Duration* | Oblika usposabljanja<br>*Degree* |
|---|---|---|---|
| Jernej Baškovč | B. Stanovnik | 2007–2012 | doktorski študij / *PhD* |
| Jure Bezenšek | B. Stanovnik | 2009–2013 | doktorski študij / *PhD* |
| Ana Bergant | J. Cerkovnik | 2004–2009 | 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* |
| 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
Damijana Urankar

## IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

### IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

### FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*
Organska kemija / *Organic Chemistry* – UN – kemija / *Chemistry*
Organska kemija II / *Organic Chemistry II* – UN – kemija / *Chemistry*

Organska kemija / *Organic Chemistry* – UN – kemijsko inženirstvo / *Chemical Engeneering*

Organska kemija / *Organic Chemistry* – UN – biokemija / *Biochemistry*

Spektroskopske metode / *Spectroscopic Methods* – UN – biokemija / *Biochemistry*

Organska kemija / *Organic Chemistry* – VS

Organska analiza / *Organic Analysis* – UN

Splošna kemija II / *General Chemistry II* – VS

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 Importnant 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 / *Study on Mechanisms of Organic Transformations*

Sodobni NMR pristopi v karakterizaciji spojin / *Modern NMR Approaches in Characterisation of Compounds*

Predbolonjski podiplomski programi / *Pre-Bologna Postgraduate Programmes*

Metode študija mehanizmov organskih reakcij / *Methods for Studying Mechanisms of Organic Reactions*

Spektroskopske metode v organski kemiji / *Spectroscopic Methods in Organic Chemistry*

Nove sintezne strategije / *New Strategies in Synthesis*

Izbrana poglavja iz organske kemije z asimetrično sintezo / *Selected Topics in Organic Chemistry Including Asymmetric Synthesis*

Kemijski in biokemijski aspekti radikalov / *Chemical and Biochemical Aspects of Radicals*

Organska fotokemija / *Organic Photochemistry*

Kemija halosubstituiranih organskih spojin / *Chemistry of Halosubstituted Organic Compounds*

Sinteza peptidov in oligonukleotidov / *Synthesis of Peptides and Oligonucleotides*

Sinteza nekaterih organskih učinkovin / *Synthesis of Some Organic Bioactive Compounds*

Izbrana poglavja iz kemije heterocikličnih spojin / *Selected Topics in Heterocyclic Chemistry*

Organska stereokemija / *Organic Stereochemistry*

Uporaba biokemijskih sistemov v organski kemiji / *The Use of Biochemical Systems in Organic Chemistry*

### 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

Predbolonjski univerzitetni podiplomski študijski programi (UPŠ Biomedicina) / *Pre-Bologna Postgraduate University Study Programme in Biomedicine*

Asimetrična sinteza / *Asymmetric Synthesis*

Kombinatorna kemija / *Combinatorial Chemistry*

## 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*

## POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

### NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- B. Stanovnik, 2009 Plaketa Tunizijskega kemijskega društva, Hammamad, Tunizija / *2009 Plaque of the Tunisian Chemical Society, Hammamad, Tunisia*
- L. Bedrač, Prešernova nagrada FKKT za leto 2009 (mentor M. A. Zupan) / *The Faculty Prešeren Award for 2009*
- J. Bezenšek, Prešernova nagrada FKKT za leto 2009 (mentor B. Stanovnik) / *The Faculty Prešeren Award for 2009*
- A. Juranovič, Prešernova nagrada FKKT za leto 2009 (mentor A. Petrič) / *The Faculty Prešeren Award for 2009*
- A. Petrič, priznanje najboljšega predavatelja na študijskem programu Biokemija v študijskem letu 2008/2009 po izboru študentov / *Students Award as the Best Lecturer on Biochemistry Study Programme in the School Year 2008/2009*
- J. Košmrlj, priznanje najboljšega predavatelja na študijskem programu Kemijska tehnologija v študijskem letu 2008/2009 po izboru študentov / *Students Award as the Best Lecturer on Chemical Technology Study Programme in the School Year 2008/2009*

### 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*

## ORGANIZACIJA MEDNARODNIH ZNANSTVENIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

V letu 2009 smo organizirali mednarodni simpozij *13th Blue Danube Symposium on Heterocyclic Chemistry*, ki je potekal od 20. do 23. septembra na Bledu. Predsednik Mednarodnega znanstvenega odbora B. Stanovnik, predsednik Organizacijskega odbora B. Stanovnik, podpredsednik Organizacijskega odbora J. Svete / *In the year 2009 we organized an international symposium* 13th Blue Danube Symposium on Heterocyclic Chemistry,*which took place from September 20 to Syptember 23, 2009 at Bled. Chairman of the International Scientific Committee B. Stanovnik, chairman of the Organizing Committee B. Stanovnik, vice-chairman J. Svete.*

## DRUGO / OTHER

- M. Kočevar je Nacionalni predstavnik v odboru (komiteju) Organic and Biomolecular Chemistry Division (III) IUPAC (za leti 2008–2009) / *Appointed a National Representative, IUPAC Organic and Biomolecular Division (III) Committee for the Period 2008–2009*
- 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 Electron Journal ARKIVOC
  d) Member of the Advisory Board “Advances in Heterocyclic Chemistry”
  e) Member of the Scientific Committee, TRAMECH, Transmediterranean Symposia of Heterocyclic Chemistry
  f) Member of the 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 Arts and Sciences, Ljubljana, Slovenia
  j) Dean of the Class for Natural Sciences, European Academy of Sciences and Arts, Salzburg, Austria in legat EASA za Slovenijo za obdobje 2010–2014.
  k) Member of the Advisory Board, Croatica Chemica Acta
  l) Member of the Advisory Editorial Board, Journal of Heterocyclic Chemistry
  m) Member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons, Den Haag, The Netherlands (1998–2004)
  n) Chairman of the Advisory Editorial Board, Vestnik Slovenskega kemijskega društva, (since 1994 Acta Chimica Slovenica) Slovenia
  o) Associate Editor, Bull. Soc. Chim. Belges, Belgium

## 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 Synthesizer 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*
- HPLC – Milton Roy / *HPLC – Milton Roy*
- HPLC – Milton Roy model 3100 / *HPLC – Milton Roy Model 3100*
- HPLC – Varian 3350 / *HPLC – Varian 3350*
- HPLC Hewlett Packard 1050 / *HPLC Hewlett Packard 1050*
- 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 ºC / *Cooler –60 ºC*
- Hidrogenator Parr / *Parr Hydrogenator*
- Avtoklavi Berghof / *Autoclaves Berghof*
- Rotavaporji Büchi / *Rotavapors Büchi*
- OptiMelt EZ (Stanford Scientific) – sistem za avtomatsko določevanje tališča / *OptiMelt EZ (Stanford Scientific) Automated Melting Point Determination System*

## **SODELOVANJE V CENTRIH ODLIČNOSTI** / CENTERS OF EXCELLENCE

Center odličnosti: Nacionalni center za NMR spektroskopijo visoke ločljivosti / *Center of Excellence: National Center for High Resolution NMR Spectroscopy*

## **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*<br>Nosilec / *Principal Researcher:* B. Stanovnik |
| P1–0230 | Organska kemija: Sinteza, struktura in aplikacija / *Organic Chemistry: Synthesis, Structure, and Application*<br>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*<br>Nosilec / *Principal Researcher:* B. Šket |
| J1–6689 | Sinteza heterocikličnih analogov aminokislin in peptidov / *Synthesis of Heterocyclic Analogs of Amino Acids and Peptides*<br>Nosilec / *Principal Researcher:* B. Stanovnik |

### **RAZVOJNI PROJEKTI** / INDUSTRIAL RESEARCH AND DEVELOPMENT

Pogodba o sodelovanju: Sinteza statinskega analoga / *Cooperation Agreement: The Synthesis of Statin Analogue*
Nosilec / *Principal Researcher:* J. Košmrlj
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju: Sinteza imunosupresanta / *Cooperation Agreement: The Synthesis of an Immunosuppressant*
Nosilec / *Principal Researcher:* J. Košmrlj
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* B. Stanovnik
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<br>*Slovenia – Argentina* | Funkcionalizacija izbranih organskih substratov in razvoj strategij za trajnostno organsko sintezo / *Functionalization of Selected Organic Substrates and the Development of Strategies for a Sustainable Organic Synthesis*<br>Nosilec / *Principal Researcher*: S. Polanc |
| Slovenija – Romunija<br>*Slovenia – Romania* | Aminokisline kot gradniki v selektivni sintezi / *Amino Acids as Building Blocks in Selective Synthesis*<br>Nosilec / *Principal Researcher*: M. Kočevar |
| Slovenija – Hrvaška<br>*Slovenia – Croatia* | Sinteza in evalvacija novih potencialnih citostatikov diazenskega tipa / *Synthesis and Evaluation of New Potential Cytostatics from Diazenes Family*<br>Nosilec / *Principal Researcher*: S. Polanc |
| Slovenija – Češka<br>*Slovenia – Czech Republic* | Nov pristop k antibakterijsko aktivnim molekulam / *New Approach to Antibacterial Active Molecules*<br>Nosilec / *Principal Researcher:* S. Polanc |

### DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

#### VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

Prof. Pierre H. Dixneuf, CNRS-Université de Rennes, Institut Sciences Chimiques de Rennes, France, *Ruthenium Catalysis in Modern Organic Synthesis: C-C Bond Formation, Heterocycles, C-H Bond Activation and Alkene Metathesis,* May 2009.

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# KATEDRA ZA ANORGANSKO KEMIJSKO TEHNOLOGIJO IN MATERIALE
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|---|---|---|---|
| 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*
- Osnove industijske kemije / *Fundamentals of Industrial Chemistry* – UN

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
- Materiali / *Materials* – VS
- Anorganski procesi in produkti / *Inorganic Processes and Products* – VS
- Osnove kemijskih tehnoloških procesov / *Fundamentals of Chemical Processes* – UN
- Anorganska kemijska tehnologija / *Inorganic Chemical Technology* – UN
- Pregled tehnologij / *Principles of Technological Processes* – UN
- Uvod v tehnologijo / *Introduction to Technology* – VS
- Kemija in kemijska tehnologija / *Chemistry and Chemical Technology* – VS
- 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

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*
- Pregled tehnologij / *Principles of Technological Processes* PEF – UN
- Industrijski materiali / *Industrial Materials* FMF – UN
- Keramika I / *Ceramics I* NTF – UN
- Gradiva / *Materials* FGG – UN in VS
- Tehnologija kovin in keramike / *Technology of Metals and Ceramics* ALU – 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; Characterisation 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

- A. Ipavec, Prešernova nagrada FKKT za leto 2009 (mentor J. Maček) / *The Faculty Prešeren Award for 2009*
- T. Marolt, Prešernova nagrada FKKT za leto 2009 (mentor M. Gaberšček) / *The Faculty Prešeren Award for 2009*
- A. Žnidaršič, Prešernova nagrada FKKT za leto 2009 (mentor M. Gaberšček) / *The Faculty Prešeren Award for 2009*
- J. Maček, Priznanje najboljšega predavatelja na študijskem programu Kemijsko inženirstvo v študijskem letu 2008/2009 po izboru študentov / *Student Award as the Best Lecturer on Chemical Engineering Study Programe in 2008/2009*
- B. Novosel, Priznanje najboljšega predavatelja na študijskem programu Varstvo pri delu in požarno varstvo v študijskem letu 2008/2009 po izboru študentov / *Student Award as the Best Lecturer on Technical Safety Study Programme in 2008/2009*

## 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 / *Scanning Probe Microscope Nanoeducator NT-MTD*

## 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*<br>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*<br>Nosilec / *Principal Researcher*: R. Dominko (KI)<br>Sofinancer / *Co-sponsored by:* Iskra TELA |

# BIBLIOGRAFIJA 2009 / REFERENCES 2009

## IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

*ATM1.* MARINŠEK, Marjan, ZUPAN, Klementina. Zgorevalna sinteza – s pomočjo gorenja do novih materialov. *Kem. šoli*, 2009, letn. 21, št. 2, str. 31–36. [COBISS.SI-ID 33518085]

*ATM2.* MARINŠEK, Marjan. Electrical conductivity of sintered LSM ceramics = Električna prevodnost sintrane LSM-keramike. *Mater. tehnol.*, 2009, letn. 43, št. 2, str. 79–84. [COBISS.SI-ID 725418]

*ATM3.* PODBRŠČEK, Peter, CRNJAK OREL, Zorica, MAČEK, Jadran. Low temperature synthesis of porous copper/zinc oxide. *Mater. res. bull.* [Print ed.], 2009, vol. 44, no. 8, str. 1642–1646. [COBISS.SI-ID 4156186]

*ATM4.* KÜZMA, Mirjana, DOMINKO, Robert, MEDEN, Anton, MAKOVEC, Darko, BELE, Marjan, JAMNIK, Janko, GABERŠČEK, Miran. Electrochemical activity of Li[sub]2FeTiO[sub4 and Li[sub]2MnTiO[sub]4 as potential active materials for Li ion batteries: a comparison with Li[sub]2NiTiO[sub]4. *J. power sources*. [Print ed.], 2009, issue 1, vol. 189, str. 81–88. [COBISS.SI-ID 4119578]

*ATM5.* KÜZMA, Mirjana, DOMINKO, Robert, HANŽEL, Darko, KODRE, Alojz, ARČON, Iztok, MEDEN, Anton, GABERŠČEK, Miran. Detailed in situ investigation of the electrochemical processes in Li[sub]2FeTiO[sub]4 cathodes. *J. Electrochem. Soc.*, 2009, vol. 156, no. 10, str. A809–A816. [COBISS.SI-ID 4219162]

*ATM6.* KASUNIČ, Marta, MEDEN, Anton, ŠKAPIN, Srečo D., SUVOROV, Danilo, GOLOBIČ, Amalija. Order-disorder of oxygen anions and vacancies in solid solutions of La[sub]2TiO[sub]5 and La[sub]4Ga[sub]2O[sub]9. *Acta crystallogr., B Struct. sci.*, 2009, vol. B65, no. 5, str. 558–566, doi: 10.1107/S010876810902833X. [COBISS.SI-ID 30821637]

*ATM7.* QIN, Ni, MAČEK, Marjeta, MEDEN, Anton, SUVOROV, Danilo. Structural investigation of K[sub]xBa[sub](1-x)-Ga[sub](2-x)Ge[sub](2+x)O[sub]8 solid solutions using the X-ray rietveld method. *J. solid state chem.*, 2009, vol. 182, no. 7, str. 1666–1672. [COBISS.SI-ID 22615591]

*ATM8.* UDOVIČ, Marko, MEDEN, Anton, SUVOROV, Danilo. Pyrochlore formation and its dielectric properties within Bi[sub]2O[sub]3-TiO[sub]2-WO[sub]3 ternary system. *Mater. sci. technol.*, 2009, vol. 25, no. 11, str. 1325–1328. [COBISS.SI-ID 23340327]

## OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI (VABLJENO PREDAVANJE) / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

*ATM9.* KOŠMERL, Tatjana, RUSJAN, Denis, FRANCETIČ, Vojmir. Negativni primeri mineralizacije v vinih = Negative examples of mineralization in wines. V: GAŠPERLIN, Lea (ur.), ŽLENDER, Božidar (ur.). 26. Bitenčevi živilski dnevi 2009 = 26th Food Technology Days 2009 dedicated to prof. F. Bitenc, 26. in 27. november 2009, Ljubljana. *Vloga mineralov v živilski tehnologiji in prehrani*. Ljubljana: Biotehniška fakulteta, Oddelek za živilstvo, 2009, str. 61–80. [COBISS.SI-ID 3722104]

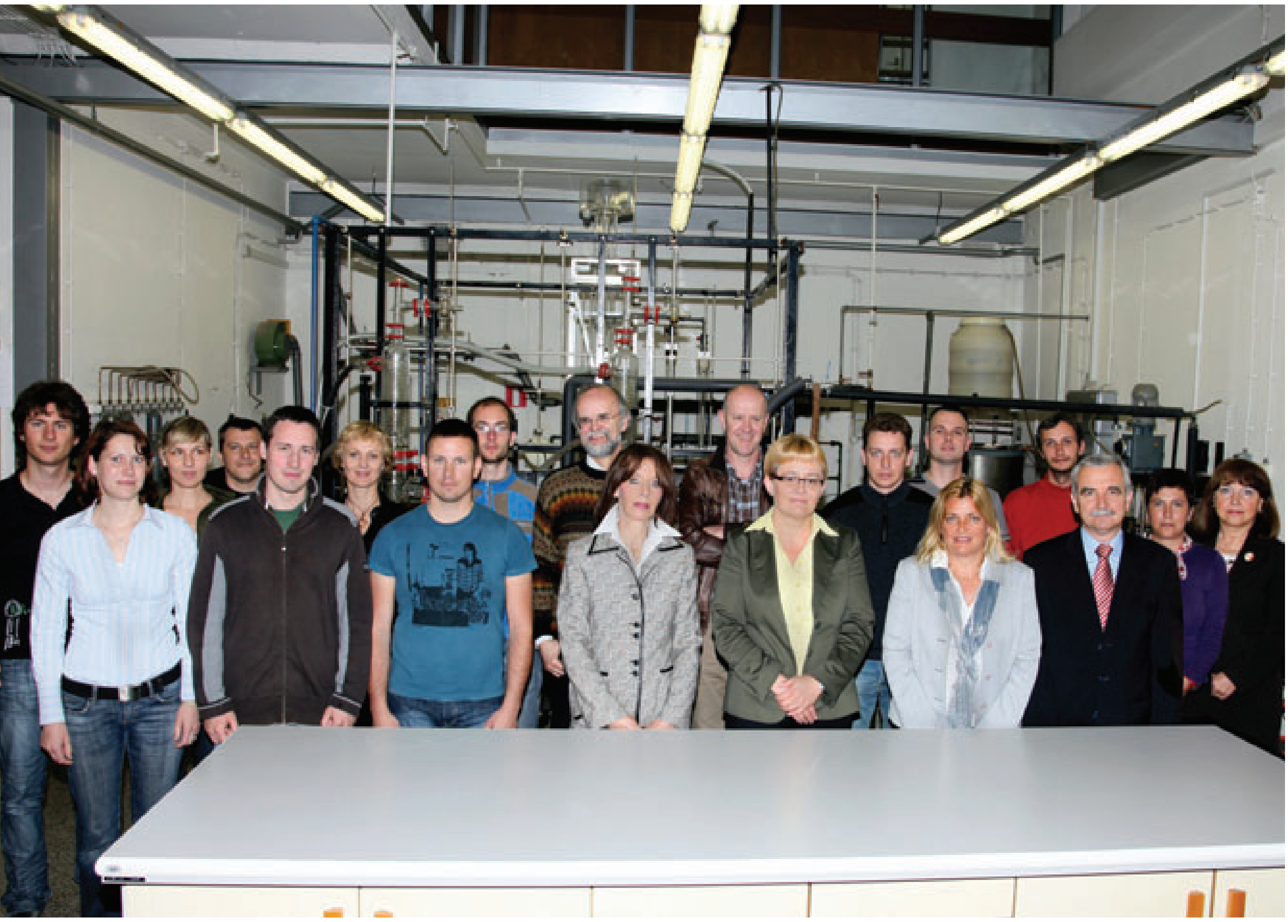
## OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

*ATM10.* DOMINKO, Robert, PEJOVNIK, Stane, GABERŠČEK, Miran. Silikati in titanati prehodnih kovin : potencialni baterijski materiali za pogon električnih avtomobilov. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2009, Maribor, 24. in 25. september 2009*. Maribor: FKKT, [2009], str. [1–8]. [COBISS.SI-ID 30845445]

## UREDNIK / EDITORSHIP

*ATM11.* MAČEK, Jadran (ur.), KOMAC, Miloš (ur.). *Študijski programi na Fakulteti za kemijo in kemijsko tehnologijo : UL FKKT*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2009. ISBN 978-961-6756-04-4. [COBISS.SI-ID 243651072]

*ATM12.* *Acta chimica slovenica*. Pejovnik, Stane (član uredniškega odbora 1998–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]



# 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
izr. prof. dr. Igor Plazl
izr. prof. dr. Jana Zagorc Končan
doc. dr. Ana Lakota Družina
izr. prof. dr. Albin Pintar (v dopolnilnem razmerju do 31. 8. 09 / *part time till 31. 8. 09)*

**Asistenti** / Assistants
doc. dr. Andreja Zupančič Valant
doc. dr. Andreja Žgajnar Gotvajn
doc. dr. Polona Žnidaršič Plazl
doc. dr. Blaž Likozar
Urban Šegedin, univ. dipl. inž. (do / *till* 30. 9. 09)

**Tehniki** / Technicians
Klemen Birtič
Vesna Delalut
Dušan Komel
Matija Matajdl, univ. dipl. inž. (od / *since* l. 12. 09)

| **Mladi raziskovalci**<br>*Young Researchers* | Mentor<br>*Mentor* | Čas usposabljanja<br>*Programme Duration* | Oblika usposabljanja<br>*Degree* |
|---|---|---|---|
| Andrej Pohar | I. Plazl | 2007–2012 | doktorski študij / *PhD* |
| Janja Babič | A. Pavko | 2005–2010 | doktorski študij / *PhD* |
| Mirjan Švagelj | M. Berovič (študijski mentor B. Štrukelj) | 2006–2011 | doktorski študij / *PhD* |
| Gorazd Stojkovič | P. Žnidaršič Plazl | 2008–2013 | doktorski študij / *PhD* |
| Matjaž Berlot | M. Berovič | 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

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
Načrtovanje procesov in naprav / *Process and Equipment Design* – VS
Kemija okolja / *Environmental Chemistry* – UN
Ekološko inženirstvo / *Environmental Engineering* – UN
Varstvo okolja / *Environmental Protection* – VS
Industrijska ekologija in ekološko inženirstvo / *Industrial Ecology and Environmental Engineering* – VS
Kemijsko procesno računstvo / *Chemical Process Calculations* – UN
Modeliranje procesov / *Process Modeling* – UN
Načrtovanje procesov in naprav / *Process and Equipment Design* – VS
Kemijsko inženirski praktikum / *Chemical Engineering Practice* – UN
Kemijsko inženirski praktikum / *Chemical Engineering Practice* – VS

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

Predbolonjski dodiplomski programi / *Pre-Bologna Undergraduate Programmes*

Procesna tehnika v živilstvu / *Food Technology* BF – UN

Bioprocesništvo / *Bioprocess Engineering* BF – UN

Zaključni procesi v biotehnologiji / *Downstream Processes in Biotechnology* BF – UN

Fizikalne, optične in kemijske metode v restavratorstvu / *Physical, Optical and Chemical Methods in Restoration and Preservation* I, II ALUO

Bolonjski programi 3. stopnje / *Bologna 3rd Cycle Doctoral Study Programmes*

Miniaturizacija bioprocesov / *Bioprocess Miniaturization* – BF

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*

Bioreaktorsko inženirstvo / *Bioreactor Engineering* – BF

Pripravljalni procesi / *Upstream Processes* – BF

Procesno integrirani sistemi / *Process Integrated Systems* – BF

Izbrana poglavja iz kemijskih in fizikalnih metod v restavratorstvu / *Chemical and Physical Methods in Restoration – Selected Topics* – ALUO

## **RAZISKOVALNA DEJAVNOST** / RESEARCH ACTIVITIES

a.) 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*

b.) 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*
  - Membranska separacija farmacevtskih učinkovin / *Membrane Separation of Pharmaceutical Compounds*

c.) Raziskave s področja okoljskega inženirstva / *Research in the Field of Environmental Engineering*
  - Integralni pristop k preprečevanju onesnaževanja voda (skupaj s Kemijskim inštitutom) / *Integrated Approach to Water Pollution Prevention* (*in Cooperation with the National Institute of Chemistry)*
  - Bioremediacija z glivami bele trohnobe / *Bioremediation with White Rot Fungi*

## POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

### NAGRADE IN PRIZNANJA / AWARDS, RECOGNITIONS

- J. Levec, Velika Preglova nagrada Kemijskega inštituta za raziskovalno delo / *The Grand Pregl Award of the National Institute of Chemistry for Research Work*

### 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 z mešalom / *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 Bioengineering AG, 2, 5,10, 15 *l* / *Laboratory Bioreactors Chemap AG, 3x* 10 *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*<br>Vodja programa / *Principal Researcher*: M. Krajnc |
| P2–0150 | Integralni pristop k preprečevanju onesnaževanja voda / *Integrated Approach to Water Pollution Prevention*<br>Vodja programa / *Principal Researcher*: A. Pintar (KI) |

## 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*<br>Nosilec / *Principal Researcher*: M. Berovič<br>Sofinancer / *Co-sponsored by*: Perutnina Ptuj |

## RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

| | |
|---|---|
| | Raziskave na področju membranskih separacijskih tehnik / *Research in the Field of Membrane Separation Techniques*<br>Nosilec / *Principal Researcher*: A. Pavko<br>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*<br>Nosilec / *Principal Researcher*: I. Plazl<br>Financer / *Sponsored by*: Trimo Trebnje d.d., Trebnje |

# MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

## BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

| | |
|---|---|
| Slovenija – Kitajska<br>*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*<br>Nosilec / *Principal Researcher*: M. Berovič |
| Slovenija – Bolgarija<br>*Slovenia – Bulgaria* | Mikrobiološke transformacije steroidov v sistemu mikrokanalov / *Microbial Transformations of Steroids within a Microchannel System*<br>Nosilec / *Principal Researcher*: P. Žnidaršič 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*
Nosilec / *Principal Researcher*: P. Žnidaršič Plazl

## VABLJENA PREDAVANJA NA INSTITUCIJAH V SLOVENIJI / INVITED LECTURES IN SLOVENIA

1. Marin Berovič, *Nove metode in tehnike procesnega inženirstva v tehnologiji pridelave vin,* Univerzitetno središče Ajdovščina, Visoka šola za vinogradništvo in vinarstvo, Ajdovščina, 20. maj 2009
2. Andreja Žgajnar Gotvajn, Boris Kompare, Jana Zagorc Končan, *Vpliv odpadnih vod avtocestnega sistema na okolje.* Vodni dnevi 2009, Portorož, 21.–22. oktober 2009
3. Polona Žnidaršič Plazl, *Kako daleč smo prišli v bioreaktorski tehniki od leta 1989 in kaj pričakujemo čez 20 let*? Posvetovanje Pomen biotehnologije in mikrobiologije za prihodnost, Ljubljana, 2.–3. december 2009

## VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

1. Prof. Dr. Luís P. Fonseca, Institute for Biotechnology and Bioengineering, Centre for Biological and Chemical Engineering, Instituto Superior Técnico, Lisboa, Portugal, *From Conventional Biosensors to New Analytical Devices for a Better Quality of Life: Magneto-Resistive Biosensors*, April 2009
2. Prof. Dr. Goran N. Jovanović, Oregon State University, Microproducts Breakthrough Institute (MBI), Corvallis, USA, *Microreactors – One Likely Future of Catalytic Chemical Processes,* December 2009

# BIBLIOGRAFIJA 2009 / REFERENCES 2009

## IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

*KIŽ1.* DJINOVIĆ, Petar, KOCJAN, Urška, BATISTA, Jurka, PINTAR, Albin. Synthesis and characterization of ordered CuO-CeO[sub]2 mixed oxides using KIT-6 silica as a hard template. *Acta chim. slov.* [Tiskana izd.], 2009, vol. 56, no. 4, str. 868–877. [COBISS.SI-ID 4337178]

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## UNIVERZITETNI ALI VISOKOŠOLSKI UČBENIK Z RECENZIJO / REVIEWED UNIVERSITY AND ACADEMIC TEXTBOOK

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## KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

*KIŽ58.* LIKOZAR, Blaž, MAJOR, Zoltan. *Characterization of fatigue crack growth behaviour of elastomer compounds : WPR-3.08-04 : project II-3.08 : failure assessment and lifetime prediction of cyclically loaded rubber compounds and composites – Part II*. Leoben: Institute of Materials Science and Testing of Plastics, University of Leoben, 2009. 58 f., ilustr. [COBISS.SI-ID 30715141]

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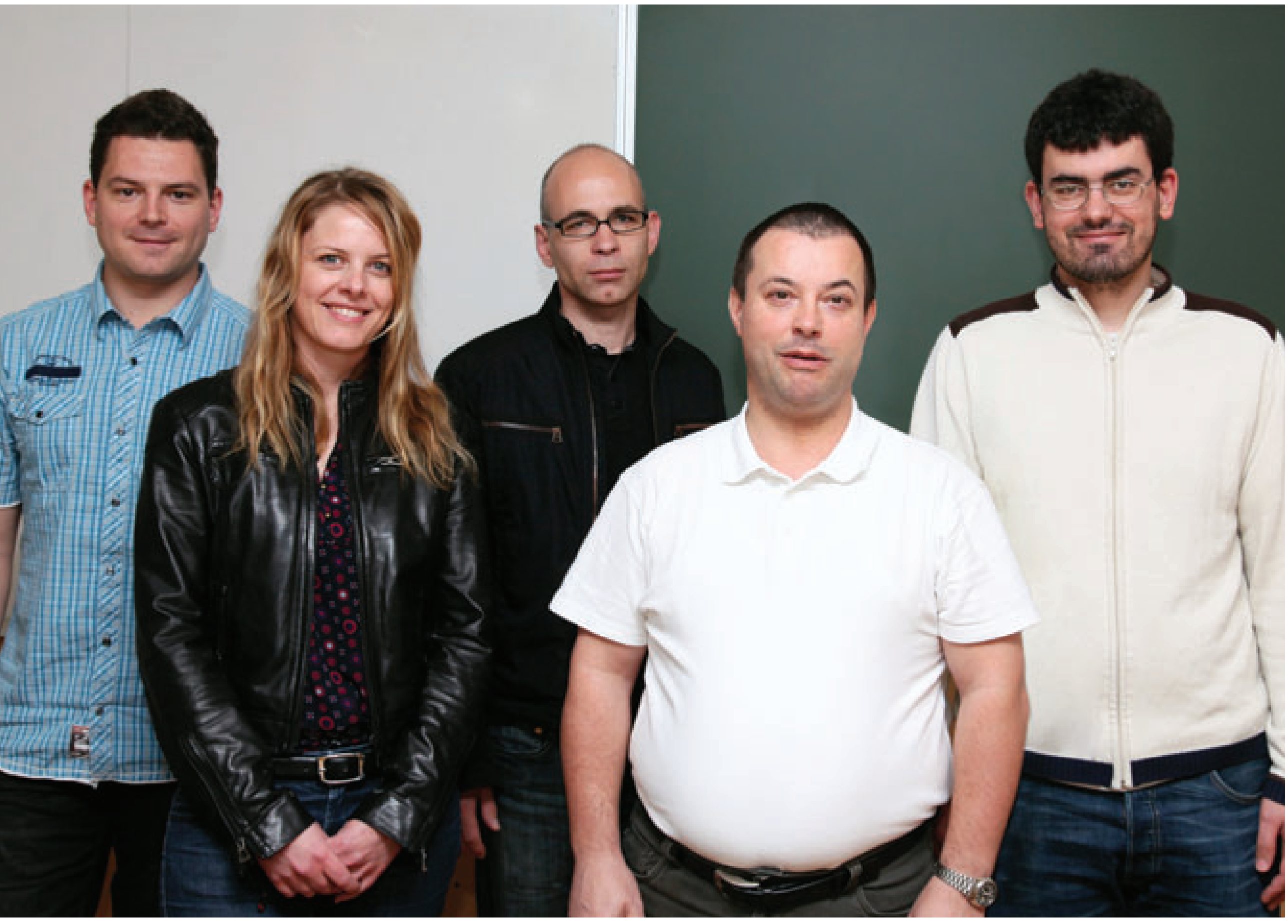

# KATEDRA ZA POLIMERNO INŽENIRSTVO, ORGANSKO KEMIJSKO TEHNOLOGIJO IN MATERIALE

## CHAIR OF POLYMER ENGINEERING, ORGANIC CHEMICAL TECHNOLOGY AND MATERIALS

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dr. Sergej Knez

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

**Tehnik** / Technician
Janez Malovrh

| **Mladi raziskovalci**<br>*Young Researchers* | Mentor<br>*Mentor* | Čas usposabljanja<br>*Programme Duration* | Oblika usposabljanja<br>*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* |

# **IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE** / EDUCATIONAL AND RESEARCH ACTIVITIES

## **IZOBRAŽEVALNA DEJAVNOST** / LECTURED COURSES

### **FKKT** / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

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
    Osnove kemijskih tehnoloških procesov / *Fundamentals of Technological Processes* – UN
    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 / *Polymer Chemistry* NTF – UN

## **RAZISKOVALNA DEJAVNOST** / RESEARCH ACTIVITIES

- Študij kinetike med vulkanizacijo različnih gumenih zmesi / *Kinetic Investigations During Vulcanization Processes of Different Rubber Blends*
- Testiranje mehanskih lastnosti gume in gumenih kompozitov / *Testing of Rubber and Rubber Composites*
- 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 melamiskih 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*

- Sinteza, priprava in karakterizacija nanokompozitnih materialov / *Synthesis, Preparation and Characterization of Nanocomposite Materials*
- 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 821e
- Mettler Toledo ReactIR iC10
- Perkin Elmer FTIR Spectrum 1000
- HP 5980II Gas Chromatograph
- LC Shimadzu LC-4A
- Microtrac S 3500 Laser Particle Size Analyzer
- Extruder Brabender Plasticorder PLD 651
- 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*<br>Vodja programa / *Principal Researcher:* M. Krajnc |
| P2–0346 | Separacijski procesi toplogrednih plinov za trajnostni razvoj / *Separation Processes of Greenhouse Gases for Sustainable Development*<br>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 formaldehidnih smol / *Research and Development of Formaldehyde Resins*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Nafta Petrochem d.o.o.

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 / *Researches in the Field of Oil Derivates*
Nosilec / *Principal Researcher*: J. Golob
Financer / *Sponsored by*: Nafta Lendava d.o.o.

# **MEDNARODNO SODELOVANJE NA PODROČJU IZOBRAŽEVANJA** / INTERNATIONAL COOPERATION IN THE FIELD OF EDUCATION

– M. Krajnc, gostujoči profesor na Fakulteti za kemijsko inženirstvo in tehnologijo, Univerza v Zagrebu / *Visiting Professor at the Faculty of Chemical Engineering and Technology, University of Zagreb*

# MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

## BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

| | |
|---|---|
| Slovenija – Ruska federacija<br>*Slovenia – Russian Federation* | Principi reoloških in mehanskih lastnosti lepil in tesnilnih mas za avtoindustrijo / *Principles of Rheological and Mechanical Properties of Adhesives and Sealants for Automotive Industry*<br>Nosilec / *Principal Researcher*: M. Krajnc |
| Slovenija – Madžarska<br>*Slovenia – Hungary* | Kompoziti guma/poliuretan/nanopolnilo: Struktura in lastnosti / *Rubber/Polyurethane/Nanofiller Systems: Structure and Properties*<br>Nosilec / *Principal Researcher*: U. Šebenik |

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*POT12.* ZIDAR, Martin, GOLOB, Janvit. Optimizacija procesov razžveplanja dimnih plinov na podlagi spremenljive surovinske osnove. 1. Del, Experimentalna simulacija SO[spodaj]2 absorpcije = Optimization of wet flue gas desulphurisation processes on the basis of changeable raw material. Part 1, Experimental simulation of SO[sub]2 absorption. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2009, Maribor, 24. in 25. september 2009*. Maribor: FKKT, [2009], str. [1–10]. [COBISS.SI-ID 30845189]

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# KATEDRA ZA VARSTVO PRI DELU
## CHAIR OF SAFETY AT WORK

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**dr. Jože Šrekl**

### SODELAVCI KATEDRE / PERSONNEL

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dr. Jože Šrekl, viš. pred.
mag. Aleš Jug, pred.
prof. dr. Stojan Petelin (v dopolnilnem razmerju / *part-time*)
doc. dr. Marija Molan (v dopolnilnem razmerju / *part-time*)

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# **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*

- Matematika I / *Mathematics* – UN
- Osnove zdravstvenega varstva / *Fundamentals of Health Care* – UN

Predbolonjski dodiplomski program / *Pre-Bologna Professional Study Programme*

- Računalništvo / *Computer Science* – VS
- Osnove varstva pri delu / *Fundamentals of Safety at Work* – VS
- Izbrana poglavja iz matematike in statistike / *Selected Topics in Mathematics and Statistics* – VS
- Varstvo okolja I / *Environmental Protection I* – VS
- Teorija gorenja, gašenja in dinamika požarov / *Theory of Combustion, Extinction and Fire Dynamics* – VS
- Delovno okolje – Prezračevanje / *Working Environment – Ventilation* – VS
- Delovno okolje – Hrup / *Working Environment – Noise* – VS
- 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 of Statistics*

# POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

## NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- Robert Šavli, Nagrada Avgusta Kuharja za najboljše diplomsko delo za leto 2009 / *The Avgust Kuhar Award for the Best Diploma Work in 2009*

## ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL MEETINGS

- Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož, maj 2009 / *Safety at Work, Fire Safety and Occupational Medicine, Two-day Symposium with International Participation, Portorož, May 2009*

# 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*<br>Nosilec / *Principal Researcher:* S. Petelin (UL FPP)<br>Sofinancer / *Co-sponsored by*: DARS d.d. – Družba za avtoceste RS |

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**POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2009**

Izdala: Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani

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