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

POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2007

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ANNUAL REPORT 2007

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KAZALO

UVODNA BESEDA

Veseli me, da prebirate Poročilo o izobraževalni in raziskovalni dejavnosti v letu 2007, ki smo ga pripravili na Fakulteti za kemijo in kemijsko tehnologijo, Univerze v Ljubljani. Poročilo smo poskušali pripraviti tako, da bi poleg potrebnih podatkov prikazali tudi vsakdanji utrip na fakulteti.

V letu 2007 smo dokončali kar nekaj zelo pomembnih aktivnosti:

1. Ustanovili smo Društvo diplomirancev UL FKKT (ALUMNI). Člani društva so lahko vsi, ki so diplomirali, magistrirali ali doktorirali na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani, oziroma na njenih predhodnicah. Konstitutivni zbor društva je bil 28. junija 2007; sprejet je bil statut društva in izvoljeni organi društva. Dr. Boris Frlec je bil izvoljen za predsednika. Vse ostale podatke najdete na naši domači strani pod rubriko ALUMNI. V kolikor še niste član Alumni Vas vabim, da to postanete in se pridružite tistim, ki želijo sodelovati pri nadaljnjem razvoju fakultete.
2. Končali smo vsebinsko razpravo o prenovi študijskih programov, skladnih z bolonjsko reformo. V letu 2008 bodo programi tudi formalno potrjeni. Tudi te prenovljene programe si lahko ogledate na naših domačih straneh. Po novih programih bomo pričeli s poukom v šolskem letu 2009–2010.
3. V sodelovanju s projektantom in vsemi sodelavci fakultete smo pripravili idejni elaborat za novo zgradbo fakultete na lokaciji Brdo. Predvidevamo, da bomo letos dobili gradbeno dovoljenje in zasadili prvo lopato. Prav gotovo bomo ob tej priložnosti pripravili družabno srečanje vseh, ki so povezani s fakulteto in upam, da boste prisotni tudi vi.

Upam, da smo s tem poročilom dokazali, da smo v letu 2007 uspešno delali ter skrbno gospodarili. Prepričan pa sem, da bomo v akademski skupnosti profesorjev, raziskovalcev, študentov in vseh ostalih sodelavcev fakultete izpolnili smele načrte, ki jih imamo za prihodnost.

Dekan:
prof. dr. Stane Pejovnik

FOREWORD

It gives me a great pleasure to present you with the Report on Educational and Research Activities in the year 2007, which has been produced by the Faculty of Chemistry and Chemical Technology at the University of Ljubljana. We have endeavoured to produce the Report in such a way that, in addition to providing the required information, it should also give an insight into the daily 'heartbeat' of our Faculty.

In 2007, we accomplished several major activities:

1. *We established the Alumni Association (ALUMNI UL FKKT). Members of this Association may all be those who have graduated, or hold master's or doctoral degrees from the Faculty of Chemistry and Chemical Technology, University of Ljubljana, or from its preceding institutions The constitutional assembly of the Association was held on June 28, 2007, at which the statute was adopted and the official bodies were elected. As President, Dr. Boris Frlec was elected. All further information may be found on our home-page under the entry ALUMNI. If you are not yet a member of the Alumni, we invite you to apply for membership and, thus, to join with those who wish to contribute towards further development of the Faculty.*
2. *We concluded the conceptual discussion on the contents of the revised study programmes in accordance with the Bologna reform, and in 2008 these programmes will also be formally approved. These programmes may also be viewed on our home-pages. Following the new programmes, instruction will begin in the academic year 2009–2010.*
3. *In collaboration with the project designers and with all associates of the Faculty, we have prepared the conceptual design for the new faculty building at the location in Brdo. We anticipate that this year we will be granted the construction permit, and then will be able to »start digging«. On this occasion, we will most surely arrange a social gathering for all of those who are associated with the Faculty – and we sincerely hope that you will also be present among them.*

I trust that this Report may assure you that, in 2007, we have indeed worked successfully and also carefully managed our affairs. I feel confident that, through the community of professors, researchers, students and all other associates of the Faculty, we shall accomplish the bold plans we have designed for the future.

Dean:
Prof. Dr. Stane Pejovnik

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, ni modernih materialov. 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 Univerza v Ljubljani.

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

FKKT izvaja 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 smermi
    - Kemijska tehnologija
    - Uporabna kemija
    - Usnjarsko predelovalna tehnologija
- visokošolski strokovni program Varstvo pri delu in požarno varstvo

FKKT izvaja tri podiplomske študijske programe:

- Kemija
- Kemijsko inženirstvo
- Kemijska tehnologija

Poleg tega pa FKKT sodeluje z drugimi fakultetami pri izvajanju naslednjih podiplomskih študijskih programov:

- Biomedicina za področje Biokemije in molekularne biologije

– Biotehnologija
– Materiali
– Varstvo okolja

Tako kot ostale članice UL, smo tudi na FKKT privzeli ECTS sistem (European Credit and Transfer System). S tem je dana osnova za prost pretok študentov med evropskimi univerzami, ki so podpisale ustrezne medsebojne bilateralne sporazume. Intenzivno pripravljamo prenovljene univerzitetne študijske programe Kemija, Biokemija in Kemijsko inženirstvo v smislu bolonjskega procesa. Odobren je bil prvostopenjski triletni univerzitetni program Tehniška varnost, ki smo ga razvili iz dosedanjega visokošolskega strokovnega programa Varstvo pri delu in požarno varstvo.

Za izvedbo študijskih programov skrbi 51 univerzitetnih učiteljev (rednih profesorjev, izrednih profesorjev in docentov), 2 višja predavatelja, 3 predavatelji, 55 asistentov, 1 višji strokovni sodelavec, 3 strokovni sodelavci ter 28 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.

VKLJUČENOST V OKOLJE

DODATNO IZOBRAŽEVANJE SREDNJEŠOLCEV IN KEMIJSKA OLIMPIADA

Na Fakulteti za kemijo in kemijsko tehnologijo se ukvarjamo tudi s srednješolci, nadarjenimi za kemijo. V sodelovanju z Zavodom RS za šolstvo organiziramo v ta namen strokovna srečanja, na katerih se dijaki dodatno izobražujejo v teoretični kemiji ter razvijajo spretnosti v laboratoriju. Srednješolci se tudi seznanijo z najnovejšimi dognanji na področju kemije, s poklicnimi možnostmi in v sklopu strokovnih ekskurzij spoznavajo inštitute in kemijsko industrijo. V februarju 2007 je začela delovati tudi modelna spletna učilnica, kjer so na voljo razne kemijske vsebine, ki so na različnih nivojih zahtevnosti. Enkrat letno pa se na neformalni prireditvi tudi srečamo vsi udeleženci tega izobraževanja: dijaki, starši, mentorji in učitelji, delavci FKKT in predstavniki ostalih inštitucij, ki so povezane z izobraževanjem v naši družbi. Gostitelj srečanja je dekan FKKT.

Na strokovnih srečanjih sicer sodelujejo učitelji in drugi sodelavci naše fakultete. Znanje srednješolcev ocenjujemo in testiramo. Med najboljšimi izberemo tudi ekipo, ki se vsako leto udeleži Mednarodne kemijske olimpiade (IChO). Srednješolci prihajajo iz različnih krajev v Sloveniji, priprave pa jim vzamejo okrog tri tedne za predavanja in vaje in še veliko prostih ur za individualni študij.

Takšno izobraževanje je povezano s stroški, zato aktivno iščemo sponzorje ali donatorje. Občasno smo v preteklih letih dobivali manjša sredstva v industriji in na Kemijskem inštitutu. V letu 2007 pa je največ razumevanja za naš projekt v Sloveniji pokazalo podjetje BASF. V četrtek, 29.3.2007 smo na Fakulteti za kemijo in kemijsko tehnologijo gostili podjetje BASF Slovenija d.o.o., ki sta ga predstavljala direktor, gospod Werner Besch in gospa Klementina Homšak. Podjetje BASF je tako postalo glavni donator slovenske dijaške ekipe, ki se je poleti 2007 udeležila kemijske olimpiade v Moskvi.

Kemijska olimpiada je tekmovanje gimnazijskih dijakov v znanju kemije. Priprave na samo olimpiado potekajo v sodelovanju z Zvezo za tehniško kulturo Slovenije na Fakulteti za kemijo in kemijsko tehnologijo. Vsako državo zastopajo po štirje dijaki in dva mentorja. Tekmovanja potekajo že od leta 1968, vsako leto v drugi državi. Poleg tekmovanja se dijaki v desetih dneh udeležijo različnih družabnih aktivnosti, ki jih organizira prireditelj olimpiade. V zadnjih letih je bila slovenska ekipa zelo uspešna. Na 39. mednarodni kemijski olimpiadi leta 2007 je sodelovalo 256 dijakov iz 66 držav. Slovensko ekipo so zastopali tekmovalci Jan Kogoj z Gimnazije Škofja Loka, Jan Bitenc z Gimnazije Bežigrad, Irena Matkovič z II. Gimnazije Maribor

in Miha Habič z Gimnazije Ljutomer, mentorja ekipe sta bila prof. dr. Darko Dolenc in dr. Andrej Godec, oba s Fakultete za kemijo in kemijsko tehnologijo. Na tem tekmovanju je naša ekipa osvojila dve srebrni (Jan Kogoj in Jan Bitenc) in eno bronasto medaljo (Irena Matkovič).

IZJEMEN USPEH NAŠIH ŠTUDENTOV BIOKEMIJE NA TEKMOVANJU V ZDA

Na tekmovanju na znameniti univerzi Massachusetts Institute of Technology (MIT) v ZDA se je ekipa študentov Univerze v Ljubljani (FKKT in BTF), v sodelovanju s Kemijskim inštitutom, z novim pristopom zdravljenja okužbe z virusom HIV uvrstila med 6 finalistov in osvojila prvo mesto med projekti s področja zdravja in medicine.

Na MIT je tretjega in četrtega novembra 2007 potekalo tekmovanje študentskih ekip z raziskovalnimi projekti na področju sintezne biologije. Tekmovanja se je udeležilo 56 ekip z vsega sveta, med katerimi so bile nekatere z najbolj uglednih ameriških, azijskih in evropskih univerz. Slovenska ekipa se je uvrstila med šest finalistov in osvojila zlato medaljo ter prvo mesto med projekti s področja zdravja in medicine.

Slovenska ekipa, ki jo je sestavljalo sedem študentov biokemije, mikrobiologije in biotehnologije s Fakultete za kemijo in kemijsko tehnologijo ter Biotehniške fakultete Univerze v Ljubljani, je pripravila projekt, v katerem so na celičnih kulturah testirali nov pristop k zdravljenju okužbe z virusom HIV, ki povzroča AIDS. Ta bolezen letno terja več kot 3 milijone življenj. Trenutno najboljša terapija HAART zaustavi razvoj AIDSa, vendar je zelo draga in je zdravila potrebno jemati do konca življenja.

Poglavitni problem zdravljenja okužbe s HIV je, da virus hitro mutira in postane odporen na zdravila, ki so usmerjana na posamezne tarče. Temu problemu so se člani slovenske ekipe izognili tako, da so namesto posameznih virusnih molekul izkoristili ključne virusne funkcije. Z eksperimentalnim delom v laboratoriju so pripravili gensko napravo, ki človeškim celicam zagotavlja obrambo pred virusom HIV, in ki ni občutljiva na virusne mutacije.

Projekt so študenti zasnovali in eksperimentalno preizkusili v petih mesecih intenzivnega raziskovalnega dela na Kemijskem inštitutu pod vodstvom petih mentorjev Laboratorija za biotehnologijo Kemijskega inštituta ter mentorja s Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani. Projekt je na tekmovanju na MIT požel veliko zanimanja in priznanja mednarodne sodniške ekipe. Rezultate projekta bo potrebno še preizkusiti na živalih, vendar obetajo, da bi lahko bili uporabni tudi za gensko zdravljenje ljudi.

Člani ekipe so bili študenti Katja Kolar, Anja Korenčič, Rok Gaber, Andrej Ondračka, Peter Cimermančič, Saša Jereb, Marko Bitenc, vodji ekipe prof. Roman Jerala in doc. Marko Dolinar, mentorji pa so bili dr. Mateja Manček Keber, dr. Mojca Benčina, Gabriela Panter in Karolina Ivičak.

NOČ ZNANSTVENIC IN ZNANSTVENIKOV 2007

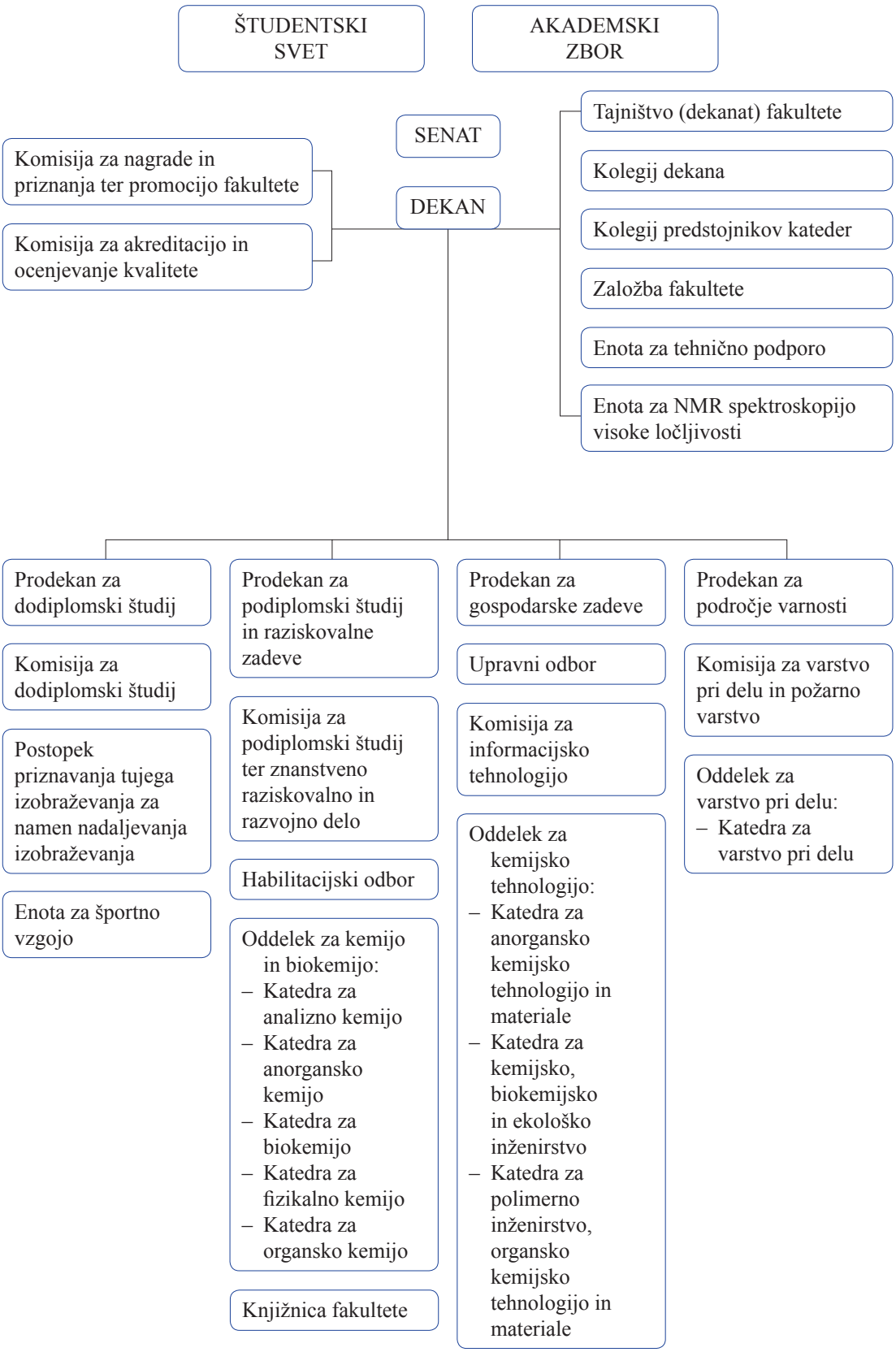
Direktorat za znanost in raziskave Evropske komisije je bil tudi v letošnjem letu pobudnik vseevropskega dogodka z imenom »Noč znanstvenic in znanstvenikov 2007«. Predhodno sta bila podobna dogodka že v letih 2005 in 2006. Bistven namen teh dogodkov je bil predvsem ta, da bi širšo laično javnost na lahkoten način seznanili z znanstvenimi dosežki. Hkrati naj bi pri mladih ljudeh vzpodbudili zanimanje za znanost in tehniko.

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 in privlačni – četudi ima veliko ljudi o znanstvenikih in njihovem delovanju prav nasprotno mnenje. Dodatne zahteve pa so bile še naslednje: v središču pozornosti naj bi bili sami znanstveniki, prišlo naj bi do spontane izmenjave mnenj med raziskovalci in obiskovalci, pa tudi obiskovalci sami naj bi sodelovali pri posameznih poskusih. Seveda naj bi se te dogodke izkoristilo tudi za popularizacijo »evropskih aktivnosti« na tem področju – predvsem 7. okvirnega programa in programov kot je npr. Marie Curie. Evropska komisija je tem aktivnostim namenila del proračuna v vrednosti 3 milijone evrov.

Temu dogodku se je pridružila tudi Fakulteta za kemijo in kemijsko tehnologijo. Podobno kot leta 2006, smo tudi v letu 2007 v lastni režiji organizirali »Noč znanstvenic in znanstvenikov 2007«. Pri organizaciji je sodelovala fakulteta, finančni del pa je pokrila programska skupina P1-0175LE. Četudi nam Evropska komisija ni dodelila sofinanciranja za izvedbo, smo pridobili status »pridruženega dogodka – *Associated Event 2007*«.

Sam dogodek je bil vezan na tematiko »Ogenj« – vse, kar ste hoteli vedeti o ognju, pa ste se bali vprašati. Predstavitev se je začela z zgodbo o Prometeju iz grške mitologije. V predavalnici fakultete smo izvedli vrsto »ognjenih« poskusov, hkrati pa prikazali tudi gašenje možnega požara z gasilnim aparatom. Posebej je bilo poudarjeno, kako pomembno je imeti doma v kuhinji kakor tudi v avtomobilu majhen priročen gasilni aparat. Tako prireditelјem kot obiskovalcem je večer ostal v prijetnem spominu.

ORGANIZACIJSKA SHEMA



DIPLOME, MAGISTERIJI IN DOKTORATI V LETU 2007

DIPLOME

UNIVERZITETNI ŠTUDIJSKI PROGRAMI

KEMIJA

Alen Albreht
Mentor: akademik prof. dr. Branko Stanovnik
Reakcije dimetilaminometilidenskega derivata etil 2-amino-4-(2-etoksi-2-oksoetil)tiazol-5-karboksilata z dušikovimi nukleofili
Datum zagovora: 19. 9. 2007

Aleksej Arko
Mentor: doc. dr. Bojan Kozlevčar
Primerjava enojedrnih in dvojedrnih bakrovih(II) spojin z anionom vanilinske kisline in N-donorskimi ligandi
Datum zagovora: 10. 7. 2007

Branko Alič
Mentor: prof. dr. Sloveko Polanc
Acilirani triazeni – priprava in lastnosti
Datum zagovora: 12. 6. 2007

Jernej Baškovč
Mentor: akademik prof. dr. Branko Stanovnik
Poskusi paralelne sinteze heterocikličnih sistemov iz dimetilaminometilidenskih derivatov acetondikarboksilatov
Datum zagovora: 30. 5.2007

Marko Bencik
Mentor: akademik prof. dr. Branko Stanovnik
Reakcije 3-amino substituiranih azolo- in azinopirimidinov z nekaterimi aldozami
Datum zagovora: 20. 9. 2007

Ana Bombač
Mentor: prof. dr. Vito Turk
Povezava cisteinskih katepsinov z apoptozo v nevroblastomski celični liniji SH-SY5Y in glioblastomski celični liniji T89G
Datum zagovora: 22. 2. 2007

Alenka Colarič
Mentor: prof. dr. Boris Pihlar
Študij interakcij Fe(III) ionov s fosfati(V) in nekaterimi karboksilatnimi ligandi
Datum zagovora: 6. 7. 2007

Ana Marija Černac
Mentorica: prof. dr. Nina Gunde-Cimerman
Učinkovitost antimikrobnih dodatkov v poliamidnem in polipropilenskem filamentu
Datum zagovora: 28. 11. 2007

Jasmina Jasna Delibašić
Mentor: doc. dr. Bogdan Štefane
Oksidacije aril- in heteroarilhidrazinov in hidrazidov z diamonijevim heksakis(nitrato-O-) ceratom(IV)
Datum zagovora: 10. 10. 2007

Kristina Eleršič
Mentorica: doc. dr. Marjanca Starčič Erjavec
Somentorica: prof. dr. Darja Žgur-Bertok
Virulentni dejavniki sevov bakterije *Escherichia coli,* izoliranih iz mešanih infekcij
Datum zagovora: 20. 6. 2007

Martin Gašper
Metorica: prof. dr. Lucija Zupančič-Kralj
Izolacija in kromatografska separacija nekaterih saponinov iz zeliščne mešanice
Datum zagovora: 7. 2. 2007

Neli Glavaš
Mentor.: prof. dr. Boris Šket
Ugotavljanje sestave organske faze sedimentov v severnem Jadranu
Datum zagovora: 4. 7. 2007

Špela Gorjan Železnik
Mentor: prof. dr. Boris Pihlar
Študij vplivov na merjenje pH z antimonskimi in polianilinskimi elektrodami
Datum zagovora: 27. 6. 2007

Darja Groznik
Mentorica: prof. dr. Lucija Zupančič-Kralj
Določevanje likopena v prehranskem dopolnilu s tekočinsko kromatografijo
Datum zagovora: 6. 7. 2007

Marjetka Jamnik
Mentorica: doc. dr. Helena Prosen
Študij ekstrakcije glikozidov iz grozdnega soka (*Vitis vinifera*) in njihove hidrolize
Datum zagovora: 29. 6. 2007

Lucija Janeš
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Določanje sestavin arome grozdja in njihovih glikozidnih prekurzorjev
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Marta Kasunič
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Koordinacijske spojine molibdena(V) in (VI) z nekaterimi
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Ksenija Kerčmar
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Slavko Klobčar
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Matrični modifikatorji v elektrotermični atomski adsorpcijski spektroskopiji
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Jasmina Koritnik
Mentorica: prof. dr. Bojana Boh
Vpliv kloriranih fenolov na rast micelija ligninolitične glive *Grifola frondosa*
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Boris Kožar
Mentor: prof. dr. Andrej Petrič
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Alenka Kralj
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Bakrove koordinacijske spojine z etanolaminom
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Aleksandra Krivec
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Določitev pomembnejših fenolnih antioksidantov v češnjah in njihova
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Robert Kulovec Müller
Mentorica: prof. dr. Bojana Boh
Študij zamreževanja alginatnih gelov za uporabo v bio-kapsuliranju
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Ana Kunej
Mentor: doc. dr. Jurij Lah
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Datum zagovora:19. 9. 2007

Andrej Lajovic
Mentor: prof. dr. Andrej Jamnik
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Barbara Lavrič
Mentor: prof. dr. Peter Bukovec
Določitev stopnje toplotne obdelave smrekovine s termogravimetrijo
Datum zagovora: 4. 10. 2007

Jure Legiša
Mentorica: doc. dr. Amalija Golobič
Struktura in sinteza zeolita ZSM-12 z uporabo tetraetilamonijevega hidroksida
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Alja Lipovšek
Mentor: prof. dr. Anton Meden
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Petra Ljubi
Mentorica: prof. dr. Brigita Lenarčič
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Jaka Marušič
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Somentor: prof. dr. Andrej Jamnik
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Luka Milivojević
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Jožef Molek
Mentor: prof. dr. Vito Turk
Somentor: prof. dr. Boris Turk
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Ana Novak
Mentor: prof. dr. Jurij Svete
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Simona Ovtar
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David Pahovnik
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Sebastijan Peljhan
Mentorica: prof. dr. Ksenija Kogej
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Darinka Primc
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Sinteze in pretvorbe enaminonskih derivatov
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Katarina Rade
Metorica: prof. dr. Ksenija Kogej
Vpliv valence protiiona na obnašanje dveh stereoizomer polimetakrilne kisline v vodnih raztopinah
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Tamara Rehar
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Bojan Šarac
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Jože Šporar
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Tina Šturm
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Gregor Trefalt
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Sabina Trošt
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Sabina Vatovec
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Nina Vidergar
Mentor: prof. dr. Vito Turk
Somentor: prof. dr. Boris Turk
Uporaba retrovirusne transdukcije za pripravo stabilnih linij celic, ki izražajo gene iz družine Cln
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Tjaša Vrlinič
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Andreja Vučkič
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Sinteza peptidomimetikov na osnovi *N*-alkiliranja (2S,4S)-4-aminopiroglutaminske kisline
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Zora Albina Zidarič
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KEMIJSKO IZOBRAŽEVANJE

Marinka Gams Petrišič
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Somentor: prof. dr. Marjan Veber
Določanje aldehidov in ketonov v zraku urbanega okolja
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Petra Kadunc
Mentorica: doc. dr. Helena Prosen
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Martin Tine Perger
Mentorica: prof. dr. Marija Bešter Rogač
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Katja Benko
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Razvoj analizne metode za določevanje amitraza in njegovih metabolitov v medu
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Anja Bubik
Mentorica: prof. dr. Tamara Lah Turnšek
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Vpliv cikličnih peptidov iz cianobakterij na proteaze in na normalne in tumorske celične linije
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Simona Fras
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Optimizacija standardne metode za določevanje pesticidov v bioloških vzorcih
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Tanja Jordan
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Delna karakterizacija nekaterih ekstracelularnih encimov pri bakteriji *Bacillus subtilis*
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Rok Kopinč
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Danijela Krgović
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Somentor: doc. dr. Aleš Podgornik
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Mitja Lah
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Špela Magister
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Vita Majce
Mentor: prof. dr. Slovenko Polanc
Somentor: prof. dr. Stanislav Gobec
Sinteza diazendikarboksamidov in njihova inhibicija D-alanin:D-alanin-ligaze
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Tanja Martinčič
Mentor: prof. dr. Jože Pungerčar
Priprava in karakterizacija rekombinantne človeške sekretorne fosfolipaze A_2 skupine V.
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Tina Tinkara Peternelj
Mentor: prof. dr. Radovan Komel
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Petra Podkrižnik
Mentor: prof. dr. Roman Jerala
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Ana Rant
Mentorica: doc. dr. Kristina Gruden
Proučevanje sprememb v proteomu prebavila koloradskega hrošča (Leptinotarsa decemlineta Say) kot odgovor na obrambni mehanizem rastline
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Marko Slana
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Martin Šala
Mentorica: prof. dr. Katja Breskvar
Somentorica: prof. dr. Vita Dolžan
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Andreja Šmerc
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Somentor: prof. dr. Peter Dovč
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Ajda Taler
Mentorica: prof. dr. Kristina Djinović Carugo
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Blaž Nemec
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Vesna Todorović
Mentorica: prof. dr. Tamara Lah Turnšek
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Barbara Zajec
Mentor: prof. dr. Radovan Komel
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Učinek različnih polimernih dodatkov na lastnosti sanacijskih malt
Datum zagovora: 1. 6. 2007

Tanja Blažič
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Submerzna kultivacija encimov *Grifole frondose*
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Vpliv hidratiziranega apna na mehanske lastnosti bitumenskih zmesi s polnilom
Datum zagovora: 16. 2. 2007

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Reološke lastnosti, notranja struktura in gostota suspenzij silike v polidimetilsiloksanu
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Dejana Dejanović
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Karakterizacija strupenosti in biorazgradljivosti odpadne fermentacijske brozge
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Klemen Dolžan
Mentorica: doc. dr. Andreja Zupančič Valant
Formulacija separacijskega gela na osnovi merjenja reoloških lastnosti in gostote
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Sebastjan Glinšek
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Marko Herga
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Vpliv procesnih pogojev na potek fermentacije vinskega mošta
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Priprava in uporaba tankih prevlek na osnovi poliedričnih oligomernih silseskvioksanov
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Masna in toplotna bilanca rotacijske peči
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Aljaž Kajtna
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Karmen Klančar
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Alen Kljajić
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Uporaba ionske kapljevine za encimsko katalizirano sintezo izoamilacetata v mikroreaktorju
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Milan Kovačević
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Tok nestisljivih tekočin v mikrokanalu
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Tilen Nastran
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David Perko
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Peter Podbrščček
Mentor: prof. dr. Jadran Maček
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Andrej Pohar
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Razgradnja odpadne fermentacijske brozge v anaerobnem reaktorju
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Maja Tinko
Mentor: prof. dr. Aleksander Pavko
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Jasmina Turnšek
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Živana Urh
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Aldijana Asanovski
Mentorica: doc. dr. Urška Šebenik
Pripava glinenih nanokompozitov s polšaržno emulzijsko polimerizacijo metilmetakrilata
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Mladen Cetina
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Tanja Čurk
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Fazne transformacije inkomenzurabilno – komenzurabilno moduliranih kristalnih struktur v oksidnih sistemih na osnovi Bi_2O_3
Datum zagovora: 20. 12. 2007

RAZISKOVALNI PROGRAMI V LETU 2007
RESEARCH PROGRAMMES IN 2007

NOSILEC / PRINCIPAL RESEARCHER	**NASLOV** / TITLE
Prof. dr. Peter Bukovec	Bioanorganska in bioorganska kemija *Bioinorganic and Bioorganic Chemistry*
Prof. dr. Boris Pihlar	Raziskave in razvoj analiznih metod in postopkov *Research and Development of Analytical Methods and Procedures*
Prof. dr. Ivan Leban	Sinteza, struktura, lastnosti snovi in materialov *Synthesis, Structure, Properties of Compounds and Materials*
Akad. prof. dr. Branko Stanovnik	Sinteze in transformacije organskih spojin. Novi reagenti v stereoselektivni in regioselektivni sintezi aminokislin kot intermediatov v organski sintezi *Syntheses and Transformations of Organic Compounds. New Reagents in Stereoselective and Regioselective Synthesis of Amino Acids as Intermediates in Organic Synthesis*
Prof. dr. Vojeslav Vlachy	Fizikalna kemija *Physical Chemistry*
Prof. dr. Marijan Kočevar	Organska kemija: sinteza, struktura, aplikacija *Organic Chemistry: Synthesis, Structure and Application*
Prof. dr. Valentin Koloini	Kemijsko inženirstvo *Chemical Engineering*
Prof. dr. Dušan Turk*	Strukturna biologija *Structural Biology*
Prof. dr. Vito Turk*	Proteoliza in njena regulacija *Proteolysis and its Regulation*
Prof. dr. Igor Križaj*	Toksini in biomembrane *Toxins and Biomembranes*
Prof. dr. Milenko Roš**	Integralni pristop k preprečevanju onesnaževanja voda *Integrated Approach to Water Pollution Prevention*

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

** Kemijski inštitut / *National Institute of Chemistry*

BIOANORGANSKA IN BIOORGANSKA KEMIJA
BIOINORGANIC AND BIOORGANIC CHEMISTRY

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0134

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Sodelujoče institucije / Participating Institutions
Institut Jožef Stefan

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Biomimetski modeli 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, kovine v okolju, nanocevke, emulzije in zelena kemija, jodiranje z elementarnim jodom, novi organski peroksidi, nove metode bromiranja

ZNANSTVENI IN DRUGI RELEVANTNI DOSEŽKI

Biomimetski modeli v bioanorganski kemiji predstavljajo enega od ciljev tega programa. Nadaljevali smo s študijem interakcij molibdenovega atoma, kot esencialnega elementa, ki ima vrsto pomembnih funkcij v živih organizmih. Pripravili smo nove komplekse tega elementa z malonovo in sukcinsko kislino in jih strukturno karakterizirali.

Okoljska problematika predstavlja aplikativni del bioanorganske kemije in zajema področja od študija speciacije kovinskih ionov z ligandi, ki jih najdemo v naravi, do procesov remediacije. Kromove soli, ki se uporabljajo v usnjarstvu, predstavljajo glavno grožnjo okolju pri odlaganju usnjarskih odpadkov na deponije. Posebno nevarne so Cr(VI) soli, ki so lahko prisotne že v odpadnih produktih usnjarske predelave, ali pa nastajajo pri oksidativnih procesih na deponiji. Zaradi preprečevanja potencialnih zdravstvenih rizikov, zakonodaja določa maksimalne dovoljene koncentracije, ne samo pri odlaganju odpadkov usnjarske industrije na depojine, temveč tudi maksimalne koncentracije Cr(VI) v usnjenih produktih. Posebno stroga je zakonodaja pri usnjenih produktih z eko-oznako. Pri spektrofotometrični določitvi Cr(VI) lahko zelo motijo druge obarvane spojine. V obširni študiji z različno obarvanimi vzorci usnja smo ugotavljali optimalni postopek za razbarvanje, ki v nadaljevanju omogoča pravilno določevanje Cr(VI) v vzorcih usnja. Ugotovili smo, da kolone polnjene s florisilom (84,0 % SiO_2, 15,5 % MgO in 0,5 % Na_2SO_4) efektivno absorbirajo vse vrste barv in omogočajo pravilno določitev Cr(VI).

Eden od praktičnih analiznih problemov, vezanih na okolju prijazne tehnologije, se nanaša na komercialna emulzijska razstreliva. Zadnja generacija komercialnih razstreliv ni več

kapsulirana, temveč se pripravlja tik pred polnjenjem v vrtine. V ta namen so potrebne hitre analizne metode, izvedljive v enem dnevu, ki omogočajo nemoteno delo na terenu. Z uporabo termogravimetrije (TG) in ciklične dinamične diferenčne kalorimetrije (DSC) smo izdelali metodo za sočasno hitro določevanje vode, amonijevega nitrata in natrijevega nitrata v emulzijah, ki se uporabljajo za pripravo razstrelilnih mešanic.

Odpadne vode, ki se težko čistijo s konvencionalnimi čistilnimi napravami, se lahko čistijo tudi z naravnimi ionskimi izmenjevalci. Z uporabo teh dodatkov sicer nastane nekoliko večja količina odpadkov, vendar je nastali produkt relativno stabilen glede na vezavo kovin. Glavna prednost pri uporabi teh materialov je predvsem nizka cena in učinkovito odstranjevanje kovinskih ionov. V prispevku je prikazana uporaba slovenskega produkta montanita 300, ki vsebuje pretežno zeolite in kremen.

Na področju materialov se naš prispevek nanaša na študij vpliva temperature na morfologijo 1D nanostruktur natrijevega titanata. Pri hidrotermalni sintezi omenjene spojine smo ugotavljali, da je specifična površina materiala odvisna od temperature sinteze. Nanocevke so nastale pri temperaturah med 115 in 135 °C, medtem ko so se nanotrakovi pojavili pri temperaturah nad 155 °C. Pri 155 °C se pojavita obe morfologiji.

Na področju organske in bioorganske kemije smo nadaljevali raziskave halogeniranja organskih spojin pod okolju prijaznimi reakcijskimi pogoji. Pokazali smo, da je mogoče organske spojine selektivno in učinkovito fluorirati tudi pod reakcijskimi pogoji brez uporabe topila. V ta namen smo uprabili dva reagenta iz skupine N-F reagentov: Selectfluor™ F-TEDA-BF_4 in Accufluor™ NFSi in na tak način uspešno transformirali celo vrsto 1,3-dikarbonilnih spojin ter aktiviranih aromatov v njihove fluorirane derivate. Prav tako smo razvili sintetsko metodo za pripravo α-bromiranih ketonov s sistemom HBr / 30 % vodni H_2O_2 v vodnem mediju. Tak pristop k bromiranju organskih molekul je podoben ustreznim procesom, ki potekajo v naravi in pomeni »zeleno« alternativo obstoječim metodam za bromiranje organskih spojin. Z obširno študijo halogeniranja ketonov z N-halo sukcinimidi pod reakcijskimi pogoji brez uporabe topila smo pokazali na procese, ki so pomembni za potek reakcije in ovrednotili njihovo vlogo pri tovrstnih transformacijah. Tako smo ugotovili, da konstante enolizacije močno vplivajo na potek reakcij, toda njihova vloga ni vedno enaka. V vrsti acetofenonov so manj enolizabilni substrati bolj reaktivni, v seriji cikličnih ketonov pa ravno obratno. Izmerili smo tudi reakcijske konstante teh reakcij in tako pokazali, da je to mogoče narediti tudi v nehomogenih reakcijskih pogojih. Odkrili in razvili smo novo metodo za aerobno jodiranje organskih molekul. Metoda je osnovana na oksidativni aktivaciji elementarnega joda z zračnim kisikom, ki je katalizirana z natrijevim nitritom. Transformacije so najbolj učinkovito in selektivno potekale v acetonitrilu kot topilu pri sobni temperaturi.

Nadaljevali smo z raziskavami na področju sinteze organskih peroksidov in novo metodo, ki uvaja uporabo 30 % vodnega H_2O_2 ob prisotnosti katalitske količine joda, aplicirali na pretvorbo različne strukturne vrste ketonov in aldehidov v geminalne hidroperokside. Z obširno študijo smo ovrednotili parametre, ki vplivajo na potek transformacije, izmerili reakcijsko konstanto za pretvorbo substituiranih benzaldehidov v geminalne hidroperokside in postulirali mehanizem reakcije.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

Studying biomimetic models 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, 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

One of the goals of the programme is to study biomimetic models in bioinorganic chemistry. We continued our research on interactions of molybdenum atom, which is an essential element with a number of functions in living systems. New complexes of molybdenum with anions of malonic and succinic acid have been prepared and structurally characterized. Applied bioinorganic chemistry refers to environmentals problems, raising from speciation of metal ions with the ligands found in the nature, to the processes of remediation. Chromium salts, used in leather industry, represent a major threat to the environment when deposited. Especially harmful are Cr(VI) salts, either present initially in leather waste products, or formed in oxidative processes in the landfill. Several legislative measures have been adopted for limiting the maximum Cr(VI) content in leather products in order to prevent health risks. For eco-labelled leather products the limits have been additionally lowered. Coloured chemical species in leather extracts may contribute to the measurement signal in spectrophotometric determination of Cr(VI). In an extensive study differently coloured leather samples were used to develop decolouring procedure, which enables a precise determination of Cr(VI) in leather samples. Florisil (84,0% SiO_2, 15,5% MgO and 0,5% Na_2SO_4) was used to remove the dyes from leather extracts prior to spectrophotometric determination of Cr(VI).

Commercial emulsion explosives have been characterised in the context of green technologies. The last generation of explosives has been prepared *on site* in bulk form, and then filled into the drilled holes just before use. For a sustainable use of explosives a quick method for quantitative characterisation has been introduced. Thermogravimetry (TG) and dynamic differential calorimetry (DSC) which operate in cyclic mode were found as most suitable methods for determining water, ammonium nitrate and sodium nitrate.

Treatment of wastewaters, containing metal ions, is often difficult by conventional procedures. While the use of natural ion exchangers may enhance the amount of waste, the waste product, however, is relatively stable regarding the binding of metal ions. The main advantages of the method are low costs of natural materials and effective adsorption of metal ions. The application of Slovenian material montanit 300, containing mainly zeolites and quartz has been presented.

In the field of materials chemistry we studied the influence of temperature on the morphology of 1D nanostructured sodium titanate. We found out that the specific surface areas of the products of hydrothermal synthesis are temperature dependant. Nanotubes were formed within the temperature range from 115 to 135 °C, while the nanoribbons were obtained at temperatures above 155 °C. However, at 155 °C both morphologies appear.

In the field of organic and bioorganic chemistry we continued our research on the application of green reaction conditions to the selective and efficient halogenation of organic compounds. We proved that the strongest single bond in organic compounds, i.e. carbon-fluorine bond, could also be formed selectively and efficiently under solvent-free reaction conditions (SFRC) using N-F electrophilic fluorination reagents: *Selectfluor*™ F-TEDA-BF_4 or *Accufluor*™ NFSi. We transformed a variety of 1,3-dicarbonyl compounds and activated aromatics into their fluorinated derivatives under SFRC using these two N-F reagents. We developed a method for the synthesis of α-brominated ketones using HBr/30% aqueous H_2O_2 in aqueous media. The method considerably mimics the corresponding natural process and represents the green alternative to known methods for the bromination of organic compounds. With an extended study on halogenation of organic compounds under SFRC using N-halosuccinimides we investigated and evaluated important parameters which regulate the reaction processes under these conditions. We established that the constants of enolisation have significant effects on the reaction course, but their role depends on the structure of ketone. In the series of acetophenones we found out that less enolisable substrates were more reactive, while in the series of cyclic ketones the effect was quite opposite. We measured reaction constants of these reactions, thus showing that such measurements could be successfully done also under SFRC. We discovered and developed a new method for aerobic iodination of organic compounds following aerobic oxidative activation of molecular iodine catalysed by sodium nitrite. The iodotransformation of organic compounds was the most efficient and selective in the MeCN solvent at room temperature.

We developed a new method for the synthesis of geminal hydroperoxides following the transformation of carbonyl functional group, using 30% aqueous H_2O_2 in the presence of catalytic amounts of molecular iodine. Thus we efficiently synthesised a variety of structural types of geminal hydroperoxides from the corresponding ketones or aldehydes. We measured the reaction constant for the transformation of substituted benzaldehydes into geminal hydroperoxides and postulated the mechanism of this reaction.

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:

1. Razvoj novih analiznih metod in postopkov
2. Raziskave procesov in parametrov, ki odločajo o lastnostih anorganskih in organskih materialov
3. Uporaba analiznih metod za meritve v industriji, okolju in prehrani

ZNANSTVENI IN DRUGI RELEVANTNI DOSEŽKI

Sodelavci programske skupine so v letu 2007 objavili 23 izvirnih znanstvenih člankov (Bibliografija katedre za analizno kemijo, *AL1–AL23*), en kratki znanstveni prispevek (*AL24*), eno vabljeno predavanje (*AL25*), 10 znanstvenih prispevkov na konferencah (*AL26–AL35*), en samostojni znanstveni sestavek v znanstveni monografiji (*AL36*), o rezultatih pa so poročali tudi na večjem številu znanstvenih simpozijev in konferenc.

Raziskovali smo naslednje:

Možnosti za uporabo modificiranega variabilnega povezovalnega indeksa prvega reda za napovedovanje pK_a vrednosti izbranih organskih kislin (*AL5*) ter s pomočjo QSPR metode, študirali kodirne sposobnosti dveh enostavnih dualističnih deskriptorjev za napovedovanje nekaterih fizikalnih lastnosti kata-kondenziranih benzenoidov (*AL16*).

Razvili smo postopek za določevanje izomer $T_{simetrične}$ fullerenheksamalonske kisline in nekaterih njenih produktov, osnovan na separaciji z ionsko izmenjevalno kromatografijo in kapilarno elektroforezo (*AL14*).

Študirali smo vpliv različnih ekstrakcijskih postopkov na učinkovitost ekstrakcije organokositrovih spojin iz sedimenta in bioloških materialov (*AL6*) in uporabnost nekaterih monolitskih nosilcev za izolacijo in delno frakcionacijo proteinov (*AL15*).

Razvili smo HPLC-MS/MS analizno metodo za izolacijo lizofosfatidnih kislin (LPA) iz plazme (*AL24*) in jo uporabili za določanje LPA v serumih pacientk z različnimi tumorji na jajčnikih (*AL11*). Pokazalo se je, da vsebnost LPA v serumu korelira s pojavnostjo tumorjev, vendar pa povišana vsebnost ne omogoča ločevanja med benignimi in malignimi oblikami tumorjev.

Pri določanju jasmonske kisline v ekstraktih *Lemna minor L.* s HPLC v kombinaciji s fluorescenčno detekcijo, smo ugotavljali merilno negotovost in identificirali ključne prispevke h končni razširjeni negotovosti merskih rezultatov (*AL1*).

Optimizirali smo pogoje za določanje hidrogenkarbonata v realnih vzorcih vod z ionsko izključitveno kromatografijo in ovrednotili rezultate glede na direktno potenciometrijo in potenciometrično titracijo v prisotnosti organskih kislin (*AL3*).

Izdelali smo nizko-cenovni spektrometrični detektor za pretočno analizo z novo optično geometrijo, ki temelji na tribarvni LED (*AL18*).

V povezavi z raziskavami na področju ohranjanja kulturne dediščine smo z metodo delnih najmanjših kvadratov primerjali spektroskopske podatke, pridobljene v bližnjem in srednjem območju infrardeče svetlobe z lastnostmi papirja, ki smo jih določili s klasičnimi kemijskimi analiznimi metodami. Na ta način smo dosegli neporušno določitev lastnosti kot so vsebnost pepela, lignina, stopnje polimerizacije, pH, ne pa vsebnosti aluminija. S tem smo pokazali, da je možno neporušno datiranje zgodovinskega papirja (*AL7*).

Preučili smo vlogo nekaterih prehodnih kovin (Fe, Cu, Mn, Co, Cr, Ni in Zn) pri oksidativni razgradnji celuloze in ugotovili, da nekatere katalizirajo nastanek hidroksilnih radikalov in s tem pospešujejo razgradnjo. Pokazalo se je, da je kemizem reakcij na papirju podoben reakcijam v raztopini (*AL17*).

S pomočjo mikroekstrakcije na trdno fazo in plinske kromatografije sklopljene z masno spektroskopijo smo pokazali, da so hlapne organske spojine, ki se sproščajo med razgradnjo papirja, pomemben vir informacij o degradaciji celuloze. Ugotovili smo, da emisije furfurala korelirajo s pH papirja, kar lahko uporabimo za neporušno določitev pH zgodovinskih dokumentov (*AL19*).

S pomočjo XANES spektroskopije smo študirali razmerja med Fe^{2+} in Fe^{3+} v zgodovinskih črnilih, kar je odločujočega pomena za korozivnost teh črnil. Ugotovili smo, da je pri tej tehniki bistvena izbira referenčnih spojin, ki morajo imeti enako simetrijo, enako lokalno strukturo in enake sosednje atome kot jih ima vzorec (*AL20*).

V monografiji (*AL36*) smo razčlenili značilnosti in uporabo kemiluminescence pri študiju razgradnje celuloze in njenih posebnosti pri raziskavah polimernih materialov, v članku (*AL21*) pa opisali možnosti uporabe vodne raztopine magnezijevega fitata za inhibicijo korozije**,** ki jo povzročajo železo-galna črnila na zgodovinskih dokumentih.

Z različnimi elektrokemijskimi tehnikami in elektrokemijsko kvarčno nanotehtnico smo študirali inhibicijo korozije bakra v prisotnosti različnih organskih inhibitorjev (*AL4*), s kombinacijo elektrokemijskih meritev in različnih spektroskopskih tehnik pa raziskovali karakteristike zaščitnih plasti nastalih na površini Cu-Zn zlitin v prisotnosti inhibitorja benzotriazola in iskali možnosti za učinkovito korozijsko zaščito teh zlitin (*AL8*).

Raziskovali smo porazdeljevanje in sorpcijo nekaterih izbranih okoljskih onesnaževal (PCB-ji, klorosubstituirani insekticidi, triazinski in amidni herbicidi) pri mikroekstakciji na trdno fazo. Iz določitve prostih koncentracij z mikroekstrakcijo na trdno fazo (SPME), smo ocenili njihovo porazdeljevanje oziroma sorpcijo v raztopljene huminske kisline (HK), na zemljo in na mineralne snovi (*AL10*).

Razvili smo ekstrakcijski postopek za analizo sestavin arome mošta in vina, osnovan na mikroekstrakciji na trdno fazo (DVB/CAR/PDMS vlakno). Analiza lahkohlapnih sestavin je potekala s plinsko kromatografijo z masno spektrometrično detekcijo (GC-MS), ekstrakt nehlapnih

komponent pa smo analizirali s tekočinsko kromatografijo v povezavi z masno spektrometrijo (LC-MS, ESI vmesnik) (*AL2*). Možnosti za identifikacijo sestavin in perspektive za uporabo tekočinske kromatografije povezane z masno spektrometrijo (LC-MS) v analitiki vina, smo opisali v članku (*AL22*). Preučili smo tudi akumulacijo bakra v 22 vinogradih v sub-mediteranskem vinorodnem področju, v povezavi z lastnostmi prsti. Pokazalo se je, da vsebnost bakra narašča s starostjo vinograda in pada z globino vzorčenja (*AL13*).

V članku (*AL12*) smo s pomočjo ^{14}C označenih spojin opazovali biogene emisije rastline *Populus tremula* in s tem povezanega potencialnega vira ogljika za mikroogranizme v okolici rastline. Proučevali smo razgradnjo označenih monoterpenov do $^{14}CO_2$ in ugotovili povezavo med hitrostjo razgradnje in oddaljenostjo od stebla rastline.

S pomočjo velikostne izključitvene kromatografije in masne spektrometrije z induktivno sklopljeno plazmo (ICP-MS) smo študirali vezavo kovin na huminske spojine v ekstraktu komposta. Po optimizaciji ICP-MS sistema in eliminaciji matričnih efektov smo ugotovili, da je delež vezave posamezne kovine na huminske spojine odvisen od molekulske mase huminskih snovi (*AL9*).

Članek (*AL23*) opisuje raziskavo vpliva emulzije PVA na izpiranje bora in bakra iz lesa ter na učinkovitost delovanja proti glivam razkrojevalkam lesa. Ugotovili smo, da dodatek PVA-emulzije izboljša vezavo borovih in bakrovih ionov v les in zavre delovanje gliv.

RESEARCH PROGRAMME REPORT

RESEARCH TOPICS AND GOALS

1. Development of novel analytical methods and procedures
2. Study of processes and parameters which determine the properties of inorganic and organic materials
3. Development of analytical methods for industrial applications, environmental analysis and food analysis

SCIENTIFIC AND OTHER RELEVANT ACHIEVEMENTS

During the last year members of the programme group published 23 original scientific papers (*AL1–AL23*), one short communication (*AL24*), one invited lecture (*AL25*), delivered ten lectures at scientific conferences (*AL26–AL35*) and had one contribution in a scientific monograph (*AL36*). The results of the research were presented at numerous scientific conferences.

The following subjects were studied:

A variable anti-connectivity topological index was optimized for the modeling of p*K*a values for selected organic acids (*AL5*). The variable anti-connectivity index of order one showed superior modeling capabilities compared to ordinary variable connectivity index of the same order because it is capable to account for the combination of positive and negative contributions for the molecular descriptor in structure-property-relationship. QSPR method was applied for determining physical properties of cata-condensed benzenoids using two simple dualist-based descriptors (*AL16*).

Ion chromatography was used to establish isomer purity of highly water-soluble sample of fullerenehexamalonic acid, $T_{h\text{-symmetric}}$ hexakis-adduct $C_{66}(COOH)_{12}$. The developed procedure can be used for the semi-quantitative determination of the extent of partial decarboxylation of the sample. As an alternative analytical technique, the capillary electrophoresis procedure was introduced and its performance against IC was compared for this particular case (*AL14*).

The efficiency of different extraction procedures for simultaneous determination of organotin compounds in mussels *Mytilus galloprovincialis* by gas chromatography – mass spectrometry was critically evaluated (*AL6*). The analytical method developed was used for determining organotin compounds in mussels from the Slovenian costal area. Butyltins, especially tributyltin, were found in mussels from all the locations investigated.

A fast and selective HPLC-MS/MS analytical method for determining different lysophosphatidic acid (LPA) species in serum as a potential biomarker for ovarian cancer has been developed and validated (*AL24*). Significantly higher total LPA levels were determined in the sera of patients with different types of tumors (benign and malignant). It was found that determination of serum LPA would be an appropriate test for ovarian tumor presence, however, the method does not provide a reliable differentiation between benign and malignant tumors (*AL11*).

In order to enable the detection of low abundance proteins from human plasma, anion-exchange chromatography using short monolithic columns prior to human plasma proteome analysis was developed (*AL15*). It has been shown that using convective interaction media monolithic columns is an efficient complementary technique for human serum albumin and immunoglobulin G removal from human plasma.

We evaluated measurement uncertainty in determining jasmonic acid content in *Lemna minor* L. plant extracts, using a reverse-phase liquid chromatography with fluorescence detection (*AL1*). The results show that the recovery method and sample homogeneity are the two main factors which contribute to uncertainty.

We determined the conditions for of hydrogen carbonate in water in the presence of (or simultaneously) with the anions of carboxylic acids by ion-exclusion chromatography was investigated (*AL3*). Optimization of the method has given the results, comparable with other traditional methods, e.g., potentiometric titration and direct potentiometry with a CO_2-responsive electrode.

A novel type of tri-colour, light-emitting, diode-based spectrometric detector for low-budget flow-injection analysis was developed (*AL18*). The LED-based detector requires optical geometry which is different from the one described in literature. The detector can be easily assembled in a laboratory with a minimum number of optical components.

Sampling restrictions in the analysis of cultural heritage materials can limit the choice of appropriate analytical methods considerably. Near- and mid-FTIR reflectance data were related to paper properties determined with classical analytical methods using partial least-squares. Non-destructive determination of properties, i.e., ash content, lignin content, degree of polymerization of cellulose, pH, could be achieved for all properties except aluminum content. Considering that chemical properties of paper change with age, nondestructive dating of historical documents was attempted for the first time (*AL7*).

Volatile organic compounds (VOCs) which are emitted from materials during degradation can be a valuable source of information. The emissions of furfural and acetic acid from cellulose were studied using solid-phase micro-extraction (SPME) in combination with gas chromatography-mass spectrometry (*AL19*). The emissions of furfural have shown correlations with the pH of the cellulosic environment and could be used for non-destructive evaluation of historical paper.

The role of some transition metals (Fe, Cu, Mn, Co, Cr, Ni, and Zn) in oxidative degradation of cellulose has been studied (*AL17*). The experiments provide strong evidence that the role of

transition metals during the oxidative degradation of cellulose is catalytic and a correlation between the behaviour of transition metals in solution and in paper was established.

The feasibility and reliability of Fe K-edge XANES spectroscopy as a tool for determining the Fe^{2+} /Fe^{3+} ratio in historic iron gall inks was investigated (*AL20*). Measurement of XANES spectra of several historic and model iron gall inks with different Fe^{2+}/Fe^{3+} ratios indicate that a proper choice of the Fe reference compounds with similar symmetry, same type of neighbour atoms in nearest coordination shells, arranged in a similar local structure is crucial for a reliable determination of Fe^{2+}/Fe^{3+} ratio in the sample.

Chemiluminometry as a tool for the characterization of cellulosic materials was reviewed and critically evaluated (*AL36*). Due to the simplicity of instrumentation and the absence of sample preparation it is a particularly attractive technique for investigating polymer degradation.

Corrosive iron ions and acids in iron gall inks lead to enhanced degradation of paper. Several conservation practices have been used to stabilise endangered documents in the past centuries. The most effective aqueous stabilisation method developed to date is the so called "Calcium phytate" method. In contribution (*AL21*) we demonstrate that treatment with magnesium phytate is equally effective and has several additional advantages.

The inhibition of copper corrosion in the presence of triazole type organic inhibitors was investigated by different electrochemical techniques and electrochemical quartz crystal nanobalance (EQCN). The results show that BTAH is a more effective inhibitor than ATA and that *in-situ* EQCN is a powerful technique for obtaining information on corrosion inhibition and its mechanism (*AL4*).

By the use of different electrochemical techniques, atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS), inhibition of brass corrosion by benzotriazole was investigated (*AL8*). It was found out that the protective surface layer formed on Cu-Zn alloys in the presence of BTAH comprised both Cu_2O and ZnO oxides, and Cu(I)-BTA and Zn(II)-BTA polymers. This film provides an effective barrier against corrosion of both metal components in a chloride solution.

Partitioning/sorption of selected environmental pollutants (PCBs, organochlorine insecticides, triazine and amide herbicides) into dissolved humic acids (HA), soil and mineral substances was evaluated by measuring their free concentrations using solid-phase microextraction (SPME) (*AL10*).

We have developed an extraction procedure for the aroma compounds from musts and wines, using solid-phase microextraction (DVB/CAR/PDMS fibre) from the headspace of heated samples. Separation and quantification of different aroma compounds (aliphatic, aromatic aldehydes, terpenes) were performed using gas chromatography – mass spectrometry and some terpene glycosides with liquid chromatography – mass spectrometry (electrospray interface) (*AL2*).

The potentials of HPLC-MS hyphenated techniques in wine analysis were reviewed (*AL22*), especially from the point of view of fermentation control and identification/quantification of numerous nonvolatile compounds such as proteins, carbohydrates, acids, and polyphenols.

Copper contamination of soil in 22 vineyards in the Sub-Mediterranean winegrowing region of Slovenia has been studied in terms of various soil properties (cation exchange capacity, organic matter and pH), vineyard age, soil depth and landform (*AL13*). Despite of the fact that Cu content in all of the studied vineyards exceeded the recommended value (60 mg/kg) it was lower than in other well-known winegrowing regions.

Decomposition of ^{14}C labelled monoterpenes, as potential carbon sources for microbial communities in soil from the rhizosphere of *Populus tremula,* was investigated (*AL12*). It was found that the evolution of $^{14}CO_2$ correlates well with the distance from the plant.

We studied the binding of metals to humic substances in compost extracts using size exclusion chromatography coupled on-line with a diode array detector and ICP-MS (*AL9*). Interferences caused by sample matrices were eliminated by the use of internal standards. The results indicate that the distribution of metals correlates with the molecular size of humic substance fractions in the compost extract.

Boron and copper compounds are very effective fungicides for wood preservation, but they leach from wood in wet environments. Influence of PVA emulsion on leaching of boron and copper from wood and efficacy on wood decay fungi was investigated (*AL23*). The results showed that addition of PVA emulsion improves copper and boron fixation and that PVA itself has a negative impact on fungal growth.

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

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

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POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

V samem predlogu raziskovalnega programa 2004–2008 smo navedli, da bomo raziskovali način priprave različnih anorganskih koordinacijskih in organokovinskih spojin z različnimi ligandi. Kemijsko čiste produkte bomo okarakterizirali s fizikalno-kemijskimi metodami in poskusili bomo določiti njihovo biološko učinkovitost. Za spojine, ki jih lahko pripravimo v obliki monokristalov, bomo določili kristalno in molekulsko strukturo z metodo rentgenske strukturne analize. Seveda pa podobne raziskave lahko opravljamo tudi s praškastimi materiali. Ker vse zgornje raziskave potrebujejo orodja rentgenske strukturne analize, bomo del raziskav posvetili tudi razvoju in uporabi teh metod. Poleg sinteze novih kemijskih spojin in materialov je študij kemijske strukture temeljna vsebina predlaganega programa. Ključna vsebina je tudi sistematična korelacija strukturnih značilnosti s fizikalnimi lastnostmi snovi (mehanskimi, optičnimi, termičnimi...), ki omogoča načrtovanje izboljšav. V časovnem poteku programa za leto 2007 smo načrtovali tudi povezovanje raziskovalne skupine v naš gospodarski prostor. To je bila predvsem tematika Katedre za anorgansko kemijo naše fakultete.

V letu 2007 smo na Katedri za anorgansko kemijsko tehnologijo in materiale del aktivnosti posvetili obvladovanju kompleksnih reakcijskih sistemov skupaj z usmerjeno pripravo materialov v produkte z načrtovanimi lastnostmi in karakteristikami.

Raziskave elektrokatalitskih materialov za visokotemperaturne sisteme gorivnih celic smo nadaljevali in jih razširili še na kompleksne keramične okside s perovskitno strukturo (LSM), ki so uporabni kot katode v SOFC gorivnih celicah. V sintezne namene smo uporabljali in izpopolnjevali postopke soobarjanja, zgorevalne sinteze in Pechini metode.

Na kompozitnih materialih Ni/YSZ tipa smo raziskovali tako procese oblikovanja takih materialov kot določali karakteristike disperzije kovine v keramični matrici in modelirali električne lastnosti tako dobljenih kompozitov. Del raziskav smo posvetili mehanizmu nastanka kompozitnega materiala iz citratno nitratnega gela, ki je potrdil, da so po sintezi faze v kompozitu porazdeljene na spodnjem nanometrskem nivoju, kar je ena od ključnih prednosti zgorevalne sinteze in jo bomo poskušali pri nadaljnem razvoju v celoti izkoristiti.

Električne lastnosti kompozitnega materiala keramika – kovina v elektrokatalizatorju za visokotemperaturne gorivne celice smo študirali v povezavi s procesom sintranja. Postopki predpriprave ter pogoji sintranja kompozita neposredno odločajo o končni gostoti komponente, s

tem pa tudi o električni prevodnosti. Del raziskav je potekal tudi na homogenem soobarjanju v sistemu bakrovi in cinkovi kationi – sečnina – voda, ki vodi do nastanka mešanih oksidov z uniformnimi velikostmi delcev.

Posebej smo študirali problematiko poogljičenja anodnih materialov za SOFC, saj le ta v precejšnji meri določa dobo uporabnosti takega materiala pod pogoji obratovanja celice z metanom ali drugimi ogljikovodiki kot gorivom.

Del raziskav je bil usmerjen na problematiko $Mo_6S_3I_6$, $Mo_6S_{4,5}I_{4,5}$ in $Mo_6S_{9-x}I_x$ nanožičk in polimernih kompozitov teh nanožičk . V tem sklopu smo študirali sintezo in karakterizacijo, tribološke lastnosti, električno prevodnost in nanomehanske lastnosti teh nanožičk.

OSREDNJE TEME PROGRAMA

Vsebina raziskovalnega programa je tako ustrezno razdeljena na dva dela. Prvi sklop programa se ukvarja s temeljnimi raziskavami, drugi sklop pa je bolj aplikativno usmerjen. V okviru raziskovalnega programa Katedre za anorgansko kemijo smo raziskovali pogoje priprave različnih anorganskih koordinacijskih in organokovinskih spojin z različnimi ligandi (**sintezni del**). Kemijsko čiste produkte smo okarakterizirali z različnimi fizikalno-kemijskimi metodami. V sklopu katedre deluje strukturni center (ki bi lahko bil center odličnosti), ki se ukvarja z rentgensko strukturno analizo tako monokristalov kot praškastih vzorcev (**strukturni del**). Rentgenski laboratorij nudi še naprej svoje usluge sodelavcem programske skupine in tudi širšemu raziskovalnemu prostoru, kakor tudi farmacevtski in drugi industriji, vendar ga bo potrebno v letu 2008 obnoviti. Iz bibliografskih podatkov katedre je razvidno, katere kristalne strukture smo obravnavali in kako so potekale raziskave (SICRIS). Raziskave tega tipa so temeljnjega značaja, vendar za nekatere spojine preverjamo tudi njihovo biološko aktivnost ter nadaljnjo možno uporabnost.

Na Katedri za anorgansko kemijsko tehnologijo in materiale smo v letu 2007 nadaljevali z raziskavami novih materialov in procesov za njihovo pripravo. Študirali smo mehanizme nastanka kompozitnih materialov, problematiko poogljičenja anodnih materialov za SOFC in posebej problematiko nanožičk in kompozitov iz nanožičk.

ZNANSTVENI DOSEŽKI

Omeniti velja zlasti naslednje dosežke:

1. Nanožičke molibden-žveplo-jod

Nanožičke z gornjo sestavo se dajo razmeroma enostavno sintetizirati, iz elementov v eni stopnji, v večjih množinah. Za karakterizacijo novega materiala na osnovi nanožičk so bile uporabljene elementna analiza, rentgenska difrakcija, termična analiza in elektronska mikroskopija. Nanožičke s to sestavo so zanimiva alternativa ogljikovim nanocevkam.

2. Različni koordinaciji ligandov v bakrovih koordinacijskih spojinah

Dve zanimivi polinuklearni bakrovi kompleksni spojini z metanoatnimi anioni in hidroksipirdinovimi ligandi sta bili sintetizirani in nedvoumno določeni z rentgensko strukturno analizo. Dodatno so bile izmerjene in razložene ustrezne magnetne lastnosti.

3. Kristalne strukture umetnih sladil – ciklamatov

V sodelovanju z Biotehniško fakulteto UL so bile določene kristalne strukture ciklamske kisline, natrijevega ciklamata, kalijevega ciklamata, amonijevega ciklamata, rubidijevega ciklamata in tetrapropilamonijevega ciklamata. Določena je bila »zwitterionska« oblika ciklamske kisline. Strukture so pomembne pri nadaljnjih, tudi fizioloških raziskavah.

DRUGI RELEVANTNI DOSEŽKI

Popularizacija znanosti

I. Leban je v letu 2007 sodeloval z enim izmed slovenskih dnevnikov, kjer je tedensko pisal prispevke z naslovom »Znanost za vse«. V njih bralcu enostavno razlaga določene naravne pojave, ki se pač dogajajo tudi v vsakdanjem življenju. Bil je tudi soorganizator vse-evropskega srečanja »Researchers Night 2007« v okviru FP7.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

The main objective on the research programme from 2004–2008 was to study various inorganic coordination and organometallic compounds with various ligands. The isolated, well-defined and pure chemical compounds were subjected to various methods of the physico-chemical analysis and some tests on biological activity have also been attempted. The crystal and molecular structure analyses were performed using X-ray analysis in cases where suitable monocrystals of the compounds were produced. However, nowadays the crystal structure analysis can be performed also on the powder samples as well. For this kind of research we employ the methods and tools for X-ray diffraction and some research time has been allocated to this subject as well. The synthesis of the new chemical substances and materials is crucial for our research. With the known crystal structures we are planning to expand our knowledge also in searching and explaining other properties correlated with the structure (mechanical, optical, thermal, stability …). The correlation between the structural and biological properties is also of fundamental importance for understanding the nature. In 2007 we explicitly focused on collaboration with industry. This part of the research was connected with the work of the Chair of Inorganic Chemistry.

In 2007 part of the research activities of the Chair of Inorganic Chemical Technology and Materials was directed into complex reaction systems and preparation of products with designed properties and characteristics.

Research of electrocatalytic materials for high temperature systems of fuel cells were continued and extended to complex ceramic oxides with perovskite structure (LSM) which can be used as cathode materials in SOFC fuel cells. Coprecipitation, combustion and Pechine methods were used for the purpose of synthesis.

We investigated the processes for the formation of composite materials of Ni/YSZ type and determined the characteristics of metal dispersion in a ceramic matrix. Electrical properties of thus prepared composites were also modelled. Part of our research was dedicated to the formation mechanism of composite materials from citrate-nitrate gel. It was confirmed that

following the synthesis, the phases of the composite are at a lower nanometer scale. This is one of the most important advantages of the combustion synthesis that we will try to further promote in the development of such materials.

We studied electrical properties of metal-ceramic composite material in the electrocatalyst for high-temperature fuel cells in relation to the process of sintering of the composite to find out that the final density of the component and the electroconductivity of the material are directly determined by the initial processes and conditions of sintering of the composite. Part of the research was also directed to homogenous coprecipitation in the system with copper and zinc cations – urea – water that led to the formation of mixed metal oxides with uniform particle sizes (after thermal treatment).

Another part of the research was focused on $Mo_6S_3I_6$, $Mo_6S_{4,5}I_{4,5}$ and $Mo_6S_{9-x}I_x$ nanowires and preparation of polymer composites with these nanowires. Synthesis, characterization, tribological properties, electrical conductivity and nanomechanical properties of nanowires were also studied.

RESEARCH TOPICS

Our research is divided into two parts: fundamental and applied research. Thus, we can say that there is a strong and modern synthetic group within the Chair of Inorganic Chemistry **(synthesis)**. Compounds are characterized by different physico-chemical methods. We managed to set up an established and well equipped structural research centre, capable of performing structural analysis of monocrystals as well as powder samples (**structure**). This X-ray laboratory offers services to various research groups in Slovenia and pharmaceutical and other chemical industries in Slovenia (A. Meden). The bibliography of the Chair, available from the SICRIS Database shows the output of our researchers in 2007. The research is mainly fundamental, with some anticipated applications.

Some new materials and processes: composites, anodic materials for SOFC and especially nanowires have been tested at the Chair of Inorganic Chemical Technology and Materials.

SCIENTIFIC ACHIEVEMENTS

1. Nanowires molybdenum-sulphur-iodine

The synthesis and characterization of new a nano-wire-like material was performed. The material can be synthesized in a single step reaction from elements in bulk quantities. The material has a fur-like appearance and is composed of nanowires that are weakly bound in bundles. Elemental analysis, X-ray diffraction, thermal analysis (TG, DTA), and electron microscopy were used for characterizing a new material in the shape of nanowires. In some applications molybdenum-sulphur-iodine nanowires seem to be an interesting alternative to carbon nanotubes.

2. Diversity of coordination ligands in copper complex compounds

Two novel polynuclear complexes with methanoate anions and 3-hydroxypyridine ligands respectively, were synthesized and characterized by X-ray structural analysis. Ferromagnetic transition was found below 20 K. This interaction probably takes place through two *syn-anti* methanoates extended in a chain through 2D structure. The other compound exhibited much weaker ferromagnetism.

3. Crystal structures of artificial sweeteners – cyclamates

A successful collaboration with Biotechnical Faculty, University of Ljubljana, led to the determination of new crystal structures of cyclamic acid, sodium cyclamate, potassium cyclamate, ammonium cyclamate, rubidium cyclamate and tetra-n-propylammonium cyclamate which were determined in the course of studying artificial sweeteners. Cyclamic acid exists in its zwitterionic form in the crystalline state. The zwitterions are connected through hydrogen bonds of the N-H ...O type to form two-dimensional sheets. The sodium, potassium, ammonium and rubidium cyclamates are isostructural.

OTHER RELEVANT ACHIEVEMENTS

Science is everywhere

Mr. I. Leban contributes regularly to the column "Science for all" in a Slovenian daily newspaper. Natural everyday phenomena are explained in a simple, reader-friendly way. The author also acted as a coordinator of the Pan-European meeting "Researchers Night 2007", an associated event within the FP7 programme.

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

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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:

S kombinatorno stereoselektivno cikloadicijo (1*Z*, 4*R**,5*R**)-1-arilmetiliden-4-benzoilamino-5-fenilpirazolidin-3-on-1-azometin iminov na *N*-substituirane maleimide smo pripravili knjižnico petnajstih 1,6,7,9-tetrasubstituiranih 6,7,9,9a-tetrahidro-5*H*-pirazolo[1,2-*a*]pirolo[3,4-*c*]-1,3,5(2*H*,3a*H*)-trionov. Ugotovili smo, da je stereokemijski potek reakcije odvisen of fenilne skupine na mestu 3 in od orto-substituent na aromatskem obroču na mestu 1´ azometin iminov. Izolirali smo dva seta diastereoizomernih cikloaduktov, prvega iz orto-nesubstituiranih dipolov, drugega pa iz orto, orto-disubstituiranih dipolov (*OK29*).

Iz etil (2*E*)-3-(dimetilamino-2-{(4*Z*)-4-[(dimetilamino)metiliden]-4,5-dihidro-5-okso-1*H*-pirazol-3il}propenoata smo z 1,2-disubstituiranimi hidrazini pripravili 2,3,5,6,7,8-heksahodropirazolo[4,3-*d*][1,2]diazepin-8-karboksilate v metanolu ali etanolu, ki se veže na intermediat, ki nato ciklizira v sedemčlenski diazepinski obroč, medtem ko nastanejo z monosubstituiranimi hidrazini derivati pirazolo[4,3-*c*]piridina (*OK9*).

Študirali smo kiralno-solvatizirajoče lastnosti (*S*)-1-benzil-6-metilpiperazin-2,5-diona, ki smo jih opazili pri sintezi derivatov indolovega alkaloida dipodazina. V devteriranem kloroformu namreč tvori enantiomerno čisti (*S*)-1-benzil-6-metilpiperazin-2,5-dion diastereoizomerne C=*O*...*H*-N asociate preko vodikove vezi z racemnim (*RS,Z*)-1-benzil-3-[(dimetilamino)m etiliden]piperazin-2,5-dionom, (*RS*)-*terc*-butil piroglutamatom in (*RS*)-*N*-benzoilalanin metil estrom. To se odraža v razcepu karakterističnih signalov v ^{1}H in ^{13}C NMR spektrih racemnih spojin. Nastanek dimer preko vodikove vezi smo študirali z ^{1}H NMR, ^{13}C NMR in 2D NMR tehnikami. S tem smo pokazali, da predstavlja ta spojina potencialni kiralno-solvatizirajoči reagent v NMR (*OK32*).

Študirali smo tudi kombinatorno sintezo v tekoči fazi (2*S*,4*S*)-4-acilamino-5-oksopirolidin-2-karboksamidov, ki smo jih pripravili preko hidroklorida di-*terc*-butil (2*S*,4*S*)-4-amino-5-

oksopirolidin-1,2-karboksilata v petih stopnjah iz (*S*)-piroglutamske kisline. Amidiranje smo izvajali s štirimi reagenti za pripajanje BPC, EEDQ, TBTU in PFTU. Od teh BPC in PFTU za nastanek karboksamidov nista primerna, ker nastanejo v glavnem diketopiperazini namesto karboksamidov (*OK15*).

S kombinatornimi cikloadicijami v tekoči fazi smo iz (1*Z*,4*R**,5*R**)-4-benzoilamino-5-fenilpirazolidin-3-on 1-azometin iminov in β-keto estrov sintetizirali knjižnico 26 bicikličnih pirazolidinonov z 6–89 % izkoristkon in 14–100 % de. Vse produkte smo izolirali z več kot 90 % čistoto. Strukturo produktov smo potrdili z NMR spektri in rentgensko analizo. Epimerizacijo cikloaduktov na anomernem C-atomu smo potrdili z ^{1}H NMR (*OK16*).

Pri reakciji (1*Z*,4*R**,5*R**)-1-arilmetiliden-4-benzamido-5-fenilpirazolidin-3-one 1-azometin iminov s kalijevim cianidom v prisotnosti ocetne kisline smo opazili, da poteka adicija HCN na eksociklično C=N vez, ki ji sledi odprtje obroča s cepitvijo N-N vezi. Pri tem nastanejo *N*-[(1*R**,2*R**)-3-amino-2-benzamido-3-okso-1-fenilpropil]benzimidoil cianidi. Struktura enega od produktov je bila potrjena tudi z rentgensko analizo (*OK28*).

Izdelali smo tudi štiristopenjsko sintezo 4-(2-aminoetil)-5-hidroksi-1*H*-pirazolov oziroma njihovih tavtomernih oblik kot pirazolske analoge histamina. Ključna stopnja v tej sintezi je kislinsko katalizirana »ring-switching« transformacija enaminolaktama z derivati hidrazina. Sinteza predstavlja novo aplikacijo enaminonske metodologije za pripravo histaminskih analogov (*OK31*).

V okviru naših prizadevanj v zvezi z enaminoni kot gradniki različnih heterocikličnih sistemov smo pripravili metil 2-(6-hidroksi-2-fenilpirimidin-4-il)acetat, ki smo ga nato uporabili kot reagent pri sintezi heteroaril substituiranih pirimidinov. Prednost te metode je v tem, da za uvedbo heteroarilnega substituenta ni potrebno uporabljati paladija (*OK8*).

Pri stereoselektivnih [3+2] cikloadicijah trimetilenmetana na eksociklične C=O in C=N vezi (1*S*,3*Z*,4*R*)-3-arilimino-1,7,7-trimetilbiciklo[2.2.1]heptan-2-onov nastanejo ustrezni derivati spiro[biciklo[2.2.1]heptan-2,2´-furana] in spiro[biciklo[2.2.1]heptan-3,2´-pirolidina]. Pri nadaljni stereoselektivni redukciji nastanejo kiralni amini, diamini in novi aminoalkoholi. Vse te reakcije potekajo samo z manj ovirane *endo*-strani (1*S*,3*EZ*,4*R*)-3-arilimino-1,7,7-trimetilbici klo[2.2.1]heptan-2-onov, tako da nastanejo ustrezni produkti s 100 % de. Strukturo produktov smo določili z NMR in NOESY spektroskopijo in rentgensko difrakcijo (*OK33*).

Študirali smo stereoselektivne »inverse-demand« [4+2]cikloadicije 3,6-bis(piridin-2-il)-1,2,4,5-tetrazin-3,6-dikarboksilata na 4´-metilendihidro-3´*H*-spiro[biciklo[2.2.1]heptan-2,2´-furan] in 4´metilen-1´-(4-ntrofenil)spiro[biciklo[2.2.1]heptan-3,2´-pirolidin]. Cikloadicije potekajo stereoselektivno na eksociklično C=C dvojno vez, pri čemer nastanejo novi derivati 11:14-isopropiliden-14-metil-2,3-diaza-8-oksadispiro[5.1.5.2]pentadekana in 11:14-isopro piliden-11-metil-2,3,8-triazadispiro[5.1.5.2]pentadekana z 50–98 % de. Strukture novih produktov smo določili z NMR in NOESY tehnikami ter rentgensko difrakcijo (*OK34*).

Nove aplisinopsinske derivate smo pripravili iz indola in 2-metilindola ter 5-dimetilaminometiliden ali etoksimetiliden-2-tiokso-1,3-tiazol-4-onov. Cikloadicija *N*-fenil-4-klorobenzonitrilimina poteče na C=S vez, tako da nastaneta spiro spojini 4,9-difenil-2-(4-klorofenil)-7-[1-(2-metilindol-3-il)metiliden]-11,6-ditia-3,4,9-triazaspiro[4.4]non-2-en-8-on in 2-(4-klorofenil)-8-[(*Z*)-1-(2-metil-1*H*-indol-3-il)metiliden]-4,6-diaril-1-tia-3,4,6,9-tetraaza-spiro[4.4]non-3-en-7-on (*OK12*).

Indolil glicinate smo z Bredereckovim reagentom pretvorili v derivate 3-[(dimetilamino)metiliden]-2,3-dihidropirazino[1,2-*a*]indol-1,4-diona, 3-(dimetilamino)-2-[(1*H*-indol-3-ilkarbonil)amino]propenoata in 2-(1-metil-1*H*-indol-2-il)-1,3-oksazol-5(4*H*)-ona, dipeptide pa v ustrezne hidantoinske derivate (*OK37*).

Skupaj s skupino z univerze v Urbinu smo izdelali regio- in stereoselektivno enostopenjsko sintezo z oksazolinskim obročem kondenziranih piridazinov s kaskadno reakcijo na osnovi

Michaelove adicijsko-piridazinske ciklizacije in oksazolinske ciklizacije 4-kloro-1,2-diaza-1,3-butadienov s 3-dimetilaminopropenoati (*OK27*).

Pregledni članek:

V tem članku smo opisali v našem laboratoriju izdelane sinteze pirazolovih derivatov s ciklizacijo alkil 2-substituiranih 3-(dimetilamino)propenoatov, alkil *E*-2-(acilamino)-3-cianopropenoatov in sorodnih enaminonov s hidrazini. Opisane so »ring-switching« reakcije pirolidin-2-onov in tetrahidrofuran-2-onov, 1,3-dipolarne cikloadicije diazoalkanov in nitril iminov na cianopropenoate in 1,3-dipolarne cikloadicije diazoalkanov na monociklične in biciklične derivate piridazinov (*OK 50*).

DRUGI RELEVANTNI DOSEŽKI

Člani programske skupine so imeli številna plenarna in vabljena predavanja na mednarodnih konferencah in na univerzah v tujini; so prejemniki uglednih nagrad in priznanj. Podrobnosti so podane v poročilu Katedre za organsko kemijo.

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:

A library of 15 1,6,7,9-tetrasubstituted 6,7,9,9a-tetrahydro-5*H*-pyrazolo[1,2-*a*]pyrrolo[3,4-*c*]pyrazole-1,2,5(2*H*,3a*H*)-triones was prepared by combinatorial stereoselective cycloadditions of (1*Z*,4*R**,5*R**)-1-arylmethylidene-4-benzoylamino-5-phenylpyrazolidin-3-on-1-azomethine imines to *N*-substituted maleimides. Stereochemistry was controlled by the stereodirecting phenyl group at position-3 and by the *ortho*-substituents at the aromatic ring at position 1´ in azomethine imines. Consequently, two sets of diastereomeric cycloadducts were obtained, one set from the *ortho*-unsubstituted dipoles and the other set from the *ortho*-disubstituted dipoles (*OK29*).

Substituted 2,3,5,6,7,8-hexahydropyrazolo[4,3-*d*][1,2]diazepine-8-carboxylates were prepared in good to excellent yields from ethyl (2*E*)-3-(dimethylamino)-2-{(4*Z*)-4-[(dimethylamino)methylidene]-4,5-dihydro-5-oxo-1*H*-pyrazol-3-yl}propenoate with 1,2-disubstituted hydrazines by heating in an alcohol (*OK9*).

In $CDCl_3$ solution, enantiopure (*S*)-1-benzyl-6-methylpiperazine-2,5-dione [(*S*)-**1a**] formed diastereomeric C=*O*·····*H*–N hydrogen bonded associates with racemic (*RS*,*Z*)-1-benzyl-3-[(dimethylamino)methylidene]piperazine-2,5-diones, (*RS*)-*tert*-butyl pyroglutamate, and (*RS*)-*N*-benzoylalanine methyl ester. This resulted in splitting (doubling) of characteristic signals in ^{1}H NMR and ^{13}C spectra of racemic compounds in the presence of one equivalent of (*S*)-**1a**. Formation of hydrogen bonded dimers in $CDCl_3$ solution was studied by ^{1}H NMR, ^{13}C NMR and 2D NMR and confirmed by the intermolecular NOE, observed between the hydrogen bonded amide protons from each of the monomeric units. On the other hand, slightly different binding mode was proposed for association of (*S*)-**1a** with alaninamide. Enantiomer compositions of known (weighed) mixures of both enantiomers of *tert*-butyl pyroglutamate were redetermined by ^{1}H NMR in the presence of of (*S*)-**1a** in $CDCl_3$. The experimental values were in good agreement with the theoretical values, thus indicating potential applicability of (*S*)-**1a** and related diketopiperazines as chiral solvating agents in NMR spectroscopy (*OK32*).

Solution-phase combinatorial synthesis of (2*S*,4*S*)-4-acylamino-5-oxopyrrolidine-2-carboxamides was studied. First, di-*tert*-butyl (2*S*,4*S*)-4-amino-5-oxopyrrolidine-1,2-dicarboxylate (hydrochloride was prepared as the key-intermediate in five steps from (*S*)-pyroglutamic acid). Acylation of the amino group followed by acidolytic deprotection gave β-(2*S*,4*S*)-4-acylamino-5-oxopyrrolidine-2-carboxylic acids, which were then coupled with amines to furnish a library of (2*S*,4*S*)-4-acylamino-5-oxopyrrolidine-2-carboxamides. Four coupling reagents, BPC, EEDQ, TBTU, and PFTU, were tested for the amidation reactions in the final step. Amidations with EEDQ and TBTU led to the desired carboxamides. On the other hand, BPC and PFTU were not suited since diketopiperazines were sometimes obtained instead of the desired carboxamides (*OK15*).

Combinatorial solution-phase cycloadditions of (1*Z*,4*R**,5*R**)-4-benzoylamino-5-phenylpyrazolidin-3-on-1-azomethine imines to β-keto esters afforded a library of 26 bicyclic pyrazolidinones in 6–89% yields and 14–100% de. All products were isolated in >90% purity according to ^{1}HNMR, and 25 of them were analytically pure. The structures of cycloadducts were confirmed by NMR and X-ray diffraction. Most of the products were isolated as mixtures of the major (1*S**,2*S**,3*R**,5*R**,6*R**)-epimers and the minor (1*R**,2*S**,3*R**,5*R**,6*R**)-epimers. Epimerization of cycloadducts at the anomeric position 1 in solution was confirmed by ^{1}H NMR (*OK16*).

Treatment of (1*Z*,4*R**,5*R**)-1-arylmethylidene-4-benzamido-5-phenylpyrazolidin-3-one 1-azomethine imines with potassium cyanide in the presence of acetic acid resulted in addition of HCN to the exocyclic C=N double bond followed by β-eliminative N-N- single bond cleavage (ring opening) to give the *N*-[(1*R**,2*R**)-3-amino-2-benzamido-3-oxo-1-phenylpropyl]benzimidoyl cyanides in 28–85% yields. Reaction of dipole with HCN furnished stable intermediate, (1´*S**,4*R**,5*R**)-4-benzamido-1-[cyano(mesityl)methyl]-5-phenylpyrazolidin-3-one in 76% yield. The structure of one compound was determined by X-ray diffraction (*OK28*).

A simple four-step synthesis of 4-(2-aminoethyl)-5-hydroxy-1*H*-pyrazoles (or their 1*H*-pyrazol-3(2*H*)-one tautomers) as the pyrazole analogues of histamine was developed. First, enamino lactam was prepared as the key intermediate in two steps from 2-pyrrolidinone. Next, acid-catalyzed »ring-switching« transformations with monosubstituted hydrazines gave *N*-[(1-substituted 5-hydroxy-1*H*-pyrazol-4-yl)ethyl]benzamides and *N*-[2-(2-heteroaryl-3-oxo-2,3-dihydro-1*H*-pyrazol-4-yl)ethyl]benzamides. Benzamides were finally hydrolysed by heating in 6 M hydrochloric acid to furnish 1-substituted 4-(2-aminoethyl)-5-hydroxy-1*H*-pyrazoles and 4-(2-aminoethyl)-2-heteroaryl-1*H*-pyrazol-3(2*H*)-ones (*OK31*).

A simple and efficient synthesis of novel 4-heteroaryl-substituted pyrimidines from 3-methyl 2-(6-hydroxy-2-phenylpyrimidin-4-yl)acetate, *via* methyl (*E*)-3-(dimethylamino)-2-(6-methoxy-2-phenylpyrimidin-4-yl)propenoate, by the enaminone methodology was developped (*OK8*).

Stereoselective [3+2] cycloadditions of trimethylenemethane (TMM) to the exocyclic C=O and C=N double bonds of (1*S*,3*EZ*,4*R*)-3-arylimino-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ones gave the corresponding spiro[bicyclo[2.2.1]heptane-2.2.0-furan] and spiro[bicyclo-[2.2.1]heptane-3,2´-pyrrolidine] derivatives. Further stereoselective reductions of the C=N or C=O bond in these cycloadducts furnished new chiral amines, diamines, and a new aminoalcohol. All cycloadditions and reductions of the C=N double bonds took place from the less hindered endo-face of the (1*S*,3*EZ*,4*R*)-3-arylimino-1,7,7-trimethylbicyclo[2.2.1]-heptan-2-ones, exclusively, thus giving the corresponding products in 100% de. The structures were determined by NMR, NOESY spectroscopy, and by X-ray diffraction (*OK33*).

Stereoselective inverse-demand [4+2] cycloadditions of 3,6-bis(pyridin-2-yl)-1,2,4,5-tetrazine and dimethyl 1,2,4,5-tetrazine-3,6-dicarboxylate to 4´-methylenedihydro-3´*H*-spiro[bicyclo[2.2.1]heptane-2,2´-furans] and 4´-methylene-1´-(4-nitrophenyl)spiro[bicyclo-

[2.2.1]heptane-3,2´-pyrrolidine] were studied. Cycloadditions took place stereoselectively at the exocyclic C=C double bonds to give novel 11:14-isopropylidene-14-methyl-2,3-diaza-8-oxadispiro[5.1.5.2]pentadecane and 11:14-isopropylidene-11-methyl-2,3,8-triazadispiro-

[5.1.5.2]pentadecane derivatives in 50–98% de. The structures of the novel dispiro compounds were determined by NMR techniques, NOESY spectroscopy and X-ray diffraction (*OK34*).

Some new thioaplysinopsin analogs were prepared from indole and or 2-methylindole and 5-dimethylaminomethylidene- or 5-ethoxymethylidene-2-thioxo-1,3-thiazol-4-ones derived from rhodanine derivatives. Cycloaddition of *N*-phenyl-4-chlorobenzonitrileimine to C=S bond in thioaplysinopsin derivatives afforded the corresponding spiro compounds 4,9-diphenyl-2-(4-chlorophenyl)-7-[1-(2-methylindol-3-yl)methylidene]-1,6-dithia-3,4,9-triazaspiro-[4.4]non-2-en-8-one and 2-(4-chlorophenyl)-8-[(*Z*)-1-(2-methyl-1*H*-indol-3-yl)methylidene]-4,6-diaryl-1-thia-3,4,6,9-tetraazaspiro[4.4]non-3-en-7-one (*OK12*).

Indolyl glycinates were transformed with *t*-butoxybis(dimethylamino)methane (Bredereck´s reagent) into 3-[(dimethylamino)methylidene]-2,3-dihydropyrazino-[1,2-*a*]indole-1,4-dione, 3-(dimethylamino)-2-[(1*H*-indol-3-ylcarbonyl)amino]propenoate, and 2-(1-methyl-1*H*-indol-2-yl)-1,3-oxazol-5(4*H*)-one derivatives. Dipeptides were transformed with Bredereck´s reagent into the hydantoin (imidazolidine-2,4-dione) derivatives (*OK37*).

In collaboration with the group at the University of Urbino a one-pot, three-step regio- and stereoselective synthesis of so far unknown functionalized oxazoline-fused pyridazines were reported. The approach involves base-assisted »Michael addition-pyridazine cyclization-oxazoline cyclization« cascade reactions of 4-chloro-1,2-diaza-1,3-butadienes with 3-dimethylaminopropenoates (*OK27*).

Review article:

In this review article the syntheses of pyrazole derivatives by cyclization of alkyl 2-substituted 3-(dimethylamino)propenoates, alkyl *E*-2-(acylamino)-3-cyanopropenoates and related enaminones with hydrazines, are described. Strategies include ring switching reactions of pyrrolidin-2-ones and tetrahydrofuran-2-ones with hydrazines, 1,3-dipolar cycloadditions of diazoalkanes and nitrile imines to 3-cyanopropenoates and 1,3-dipolar cycloadditions of diazoalkanes to monocyclic and bicyclic pyridazine derivatives (*OK50*).

OTHER RELEVANT ACHIEVEMENTS

Members of the programme group delivered several plenary and invited lectures at international conferences and foreign universities. They are recipients of prestigious awards. Details can be found in the report of the Chair of Organic Chemistry.

FIZIKALNA KEMIJA
PHYSICAL CHEMISTRY

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0201

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POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Cilji naših raziskav so prispevati k razumevanju fizikalno-kemijskih procesov, ki se dogajajo v živih bitjih ali pa so pomembni v industriji. Zanimajo nas predvsem raztopine in suspenzije nanodelcev. Nekateri med njimi so biološko pomembni (proteini in DNK), drugi, na primer, koloidi, površinsko aktivne snovi in polielektroliti pa se na široko uporabljajo v industriji. Naše raziskave naj bi, ob pomoči najnovejših merskih in teoretičnih metod ter računalniških simulacij, obogatile osnovna znanja na področju fizikalne in biofizikalne kemije. Zelo pomembno mesto v znanosti in tehnologiji imajo raztopine nizkomolekularnih in polimernih elektrolitov. Ioni, tako preprosti kot bolj zapleteni, sodelujejo v življenjsko pomembnih procesih v našem telesu. Voda kot najpomembnejše topilo igra pri tem vlogo, ki še zdaleč ni v celoti razumljena. Primer so tako imenovane »hidrofobne interakcije«, o njih so napisane mnoge knjige, a mnenja o tem, kako in zakaj nastanejo, so različna. Raziskave stabilnosti proteinov in DNK, vezave ligandov na DNK in podobnosti molekul so pomembne v farmacevtski industriji in bioinženirstvu; prav na teh področjih sodelujemo tudi z industrijo. V ekologiji in pri separacijskih procesih pa je pomembno poznavanje lastnosti polielektrolitov, interakcij med njimi in površinsko aktivnimi snovmi ter s kovinskimi protiioni. Eksperimentalne raziskave se dopolnjujejo s teoretičnimi; namen našega dela je razumevanje fizikalno−kemijskih procesov na molekularnem nivoju.

OSREDNJE TEME PROGRAMA

1. Raziskave elektrolitov in polielektrolitov
   – Transportne in strukturne lastnosti vodnih raztopin fulerenskih elektrolitov
   – Solvatacija večvalentnih ionov
   – Termodinamične in transportne lastnosti stereoregularnih polielektrolitov
   – Fizikalno-kemijske raziskave raztopin ionenov z različnimi protiioni

- Termodinamične in transportne lastnosti soli polianetolesulfonske kisline
- Interakcije površinsko aktivnih snovi s polielektroliti

2. Lastnosti raztopin biološko pomembnih molekul
   - Termodinamika molekulskega prepoznavanja biološko pomembnih molekul.
   - Termodinamska stabilnost in interakcije biološko pomembnih molekul v povezavi z njihovimi strukturnimi značilnostmi
   - Termodinamične in strukturne lastnosti raztopin proteinov HSA in lizocima
3. Raziskave strukturnih lastnosti koloidnih disperzij ter različnih mikroemulzij in gelov
4. Teoretične raziskave vodnih raztopin
   - Dinamika ionov v neurejeni porozni snovi
   - Lastnosti vode v zaprtih in nehomogenih sistemih
   - Modeli vode in raziskave hidratacije preprostih in polimernih topljencev.
   - Dvodelčne porazdelitvene funkcije ionov v okolici valjastega poliiona. Katalitični efekt
   - Vpliv dielektrične nezveznosti na lastnosti vodnih raztopin micelov
   - Mešanice modelnih tekočin z adhezivnim privlačnim medmolekulskim potencialom

ZNANSTVENI DOSEŽKI

V letu 2007 smo objavili 35 člankov (eden je pregledni), večji del v zelo uglednih revijah. Izbrali smo tri članke, ki ilustrirajo naše raziskave. Poleg teh so enako pomembne še raziskave objavljene v delih pod zaporedno št. FK 16, 20, 27 in 35.

FK29: S pomočjo velekanonične simulacije Monte Carlo in z replika Ornstein−Zernike teorijo, ki smo jo razvili v prejšnjih letih, smo proučevali strukturne in termodinamične lastnosti modelne raztopine simetričnega elektrolita v neurejeni nabiti porozni snovi. Slednjo smo si zamislili kot neko ravnotežno razporeditev negativno nabitih togih kroglic. Prosti protiioni in koioni so bili nato razporejeni v takšen adsorbent, ki je bil v termodinamičnem ravnovesju z zunanjim rezervoarjem enakega elektrolita. Simulacije smo izvajali za vrsto parametrov, pri čemer smo spreminjali neto naboj adsorbenta in adsorbiranega elektrolita, prav tako pa smo spreminjali tudi dielektrično konstanto medija. Koncentracija adsorbiranega elektrolita je bila manjša kot v zunanji nemoteni raztopini in je bila odvisna od dielektričnosti medija ter od koncentracije vseh ostalih komponent. Najpomembnejši vpliv na vedenje elektrolita pa je imel neto naboj adsorbenta. Ujemanje napovedi teorije s simulacijami je izredno dobro. Takšne študije so pomembne za boljše razumevanje procesov v heterogenih sistemih.

FK30: Lastnosti polielektrolitov so lahko močno odvisne od strukture polimerne verige na mikroskopskem nivoju, to je od njihove stereoregularne sestave ali t.i. taktičnosti. Vpliv stereoregularnosti na lastnosti nevtralnih polimerov v organskih topilih je znan, zelo pomanjkljivo pa je znanje o povezavi med mikrostrukturo in lastnostmi poliionov v vodnih raztopinah. V tem delu smo proučevali vpliv taktičnosti na vezanje protiionov in na navidezne molske volumne v vodnih raztopinah polimetakrilne kisline, PMA. Izbrali smo tri stereoizomere PMA, izotaktično, sindiotaktično in ataktično oblike, i-PMA, s-PMA in a-PMA. Osmozni koeficienti kažejo, da so natrijevi ioni najmočneje vezani ob poliion i-PMA, medtem ko volumni skupaj z meritvami sipanja kažejo na močno asociacijo med verigami i-PMA pri ioniza-

ciji karboksilnih skupin na poliionu pod 50 %. Kratke verige i-PMA in s-PMA smo študirali s semiempirično metodo na osnovi metode molekulskih orbital in pokazali, da so razlogi za to večja gostota naboja, bolj toga veriga ter, v primeru i-PMA, lokalna struktura vijačnice.

FK32: Izmerili smo električno prevodnost razredčenih vodnih raztopin penicilin G natrijeve in kalijeve soli ter penicilin V kalijeve soli v temperaturnem območju med 278.15 in 313.15 K. Z uporabo Quint−Viallardovih zvez za električno prevodnost raztopin smo določili konstante disociacije soli ter limitne vrednosti prevodnosti penicilin aniona. Izkazalo se je, da obravnavane soli v vodni raztopini kažejo lastnosti kislih soli dvobaznih kislin, ki so končni produkti razgradnje penicilina v kislih medijih.

DRUGI RELEVANTNI DOSEŽKI

- V. Vlachy (gostujoči urednik), M. Bešter Rogač (gostujoča urednica), *J. Mol. Liq*. 2007, vol. 131/132, Amsterdam, Elsevier
- V. Vlachy, gostujoči profesor, Univerza v Regensburgu, 15. 10. 2006–14. 4. 2007
- V. Vlachy, gostujoči profesor, Univerza Pierre in Marie Curie, Pariz, 15. 5–15. 6. 2007
- V. Vlachy, vabljeno predavanje, *Modelling Charged Macromolecules in Solution*, European Polymer Congress, Portorož, Slovenija, julij 2007
- V. Vlachy, vabljeno predavanje, *Polyelectrolyte Hydration: Theory and Experiment*, 30th International Conference on Solution Chemistry, Perth, Avstralija, julij 2007

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

The main goal of our research is to contribute toward better understanding of the physico−chemical processes in living beings or/and technologically important processes. We focus on nanoparticles in solutions. Some of them, e.g. proteins and DNA, are of biological importance, the others, e.g. colloids, surfactants, polyelectrolytes are used in industrial application. Using advanced measuring techniques and theoretical methods, including computer simulations, we are striving to enrich basic knowledge in the fields of physical chemistry. There is no doubt that electrolyte and polyelectrolyte solutions play an important role in science and technology. Simple, as well as complex ions are part of the processes in living beings. Water, being by far the most important solvent, plays a central role in these processes, and yet its role is not completely understood on the molecular level. For example, many books have been written on hydrophobic effect, but its mechanism has still not been unambiguously explained. Studies of protein and DNA stability are invaluable for pharmaceutical industry and bioengineering. For ecology and separation processes it is of vital importance to know the properties of polyelectrolytes and to understand their interaction with surfactants and metal ions. Wherever possible, the experimental research is complemented with theoretical analysis; the main purpose of our work is to understand the physico-chemical processes on the molecular level.

RESEARCH ACTIVITIES

1. Research of electrolytes and polyelectrolytes
   - Transport and structural properties of aqueous solutions of fullerene electrolytes
   - Interactions of multivalent ions with a solvent
   - Thermodynamic and transport properties of different stereoregular polyelectrolytes
   - Thermodynamic and transport properties of ionene solutions with different counter ions
   - Study of polyanetholesulfonic acid and its alkaline salts
2. Properties of solutions of biologically important molecules
   - Thermodynamics of molecular recognition of biologically important molecules
   - Thermodynamic stability and interaction of biologically important molecules and correlation with their structural properties
   - Thermodynamic and structural properties of protein solutions
3. Studies of structural properties of colloid dispersions, microemulsions and gels
4. Theoretical studies of aqueous solutions
   - Electrolyte adsorption in disordered materials: dynamics and structure
   - Properties of water in confined and inhomogeneous systems
   - Modeling water and solvation of simple solutes
   - Ion correlations in the inhomogeneous atmosphere surrounding cylindrical polyions
   - Potential of mean force between charged colloids: effect of dielectric discontinuities
   - Mixtures of model liquids. Molecules with adhesive intermolecular potential

SCIENTIFIC ACHIEVEMENTS

In 2007, 35 papers were published, including one review paper. Most of them appeared in journals with high SCI. Below we selected three of them. We believe these three publications illustrate our work accomplished in the past year. Equally important are the articles denoted by FK 16, 20, 27 in 35.

FK29: Structural and thermodynamic properties of the restrictive primitive model +1:-1 electrolyte solution adsorbed in a disordered charged media were studied by means of the Grand Canonical Monte Carlo simulation and the replica Ornstein-Zernike theory. Disordered medium was represented by a distribution of negatively charged hard spheres frozen in a particular equilibrium distribution. The annealed ions were assumed to be distributed within the nanoporous adsorbent in thermodynamic equilibrium with an external reservoir of the same electrolyte. The simulations were performed for a set of model parameters, varying the net charge of the matrix and of annealed electrolyte, in addition to the dielectric constant of the invading solution. The concentration of adsorbed electrolyte was found to be lower than the corresponding concentration of the equilibrium bulk solution. The "exclusion" strongly depended on dielectric constant of the media as also on the concentrations of all other components. The most important parameter was the net charge of the matrix. The agreement between the predictions of the theory with the exact simulation results was very good. Such studies are important for better understanding of the processes in heterogeneous systems.

FK30: We have determined osmotic coefficients and apparent molar volumes of three stereoisomers of polymethacrylic acid, PMA, in aqueous solutions: isotactic, syndiotactic and atactic form, i-PMA, s-PMA, and a-PMA, respectively (1). Osmotic coefficients indicate that sodium ions are most strongly bound to i-PMA, whereas the volume and light-scattering results point to strong intermolecular association between i-PMA chains at degrees of ionization below 50%. A molecular dynamics study revealed that the observed behavior can be attributed to larger charge density, greater rigidity and local helical structure in the case of the i-PMA chain.

FK32: Systematic determinations of electrical conductivities of sodium penicillin G, potassium penicillin G, and potassium penicillin V in the 278.15–313.15 K temperature range are reported. These conductivities are examined by applying the Quint-Viallard conductivity equations.Determined dissociation constants and the limiting conductances of penicillin anions are based on the assumption that in dilute aqueous solutions, penicillin salts behave as acidic salts of dibasic acids, which are the final products of degradation reactions in acidic media

OTHER RELEVANT ACHIEVEMENTS

- V. Vlachy (Guest Editor), M. Bešter Rogač (Guest Editor), *J. Mol. Liq.* 2007, vol. 131/132, Amsterdam, Elsevier
- V. Vlachy, Visiting Professor, University of Regensburg, 15. 10. 2006–14. 4. 2007
- V. Vlachy, Visiting Professor, Universite Pierre&Marie Curie, Paris, 15. 5–15. 6. 2007
- V. Vlachy, Invited Talk, *Modelling Charged Macromolecules in Solution*, European Polymer Congress, Portorož, Slovenia, July 2007
- V. Vlachy, Invited Talk, *Polyelectrolyte Hydration: Theory and Experiment,* 30th International Conference on Solution Chemistry, Perth, Australia, July 2007

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

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P1–0230

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POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Naš cilj je razvijati sinteze spojin za znanstvene in aplikativne namene pod okolju čim bolj prijaznimi pogoji (zelena kemija) in z visoko atomsko ekonomičnostjo.

OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

V okviru projekta COST D24/007 smo razvijali nove metode za sintezo in hidrogeniranje sterično oviranih heteropolicikličnih derivatov biciklo[2.2.2]oktena. Dvojno Diels−Alderjevo reakcijo serije 2*H*-piran-2-onskih derivatov in *N*-substituiranih maleimidov, pri kateri nastanejo ustrezni biciklo[2.2.2]okteni, smo izvajali pod zelenimi pogoji v vodi kot topilu ter pod pogoji obsevanja z mikrovalovi. Tako pripravljeni produkti so služili za raziskavo heterogenega hidrogeniranja z uporabo ionskih imobiliziranih kompleksov Rh na LDH (layered double hydroxide) podlagi. Za pripravo katalizatorja smo uporabili $[Rh(cod)Cl]_2$ (kot vir rodijevih ionov), hidrokside Zn_3AlCl in Co_2FeCO_3 (kot LDH) ter dva vodotopna liganda: trinatrijev trifenilfosfin-3,3′,3′′-trisulfonat (TPPTS) in litijev trifenilfosfin-3,3′,3′′-trikarbonat (*m*-TPPTC). Tako pripravljene katalizatorje je mogoče regenerirati in ponovno uporabljati brez znatne izgube selektivnosti. Bistvo raziskav je predstavljala optimizacija katalizatorja Rh/TPPTS/LDH za hidrogeniranje naših substratov in sama izvedba hidrogeniranja. K sodelovanju smo pritegnili še skupino iz univerze v Salamanci, Španija. Karakterizacija katalizatorja je bila izvedena z uporabo več tehnik: kemijsko sestavo smo ugotavljali z ICP atomskim emisijskim spektrometrom; N_2 adsorpcijsko-desorpcijsko izotermo smo merili pri −196 °C z Micromeritics ASAP 2020; poslužili smo se tudi praškovne rentgenske analize itd. Naši rezultati so pokazali, da so sterično ovirani substrati inertni za hidrogeniranje s klasičnimi katalizatorji, da pa jih je možno hidrogenirati z uporabo ionskih imobiliziranih kompleksov Rh-ligand na LDH (*OK17*).

Diels−Alderjevo reakcijo *2H*-piran-2-onov s serijo *N*-substituiranih maleimidov do derivatov biciklo[2.2.2]oktena, ki smo jo izvajali pod mikrovalovnimi pogoji kot »neat reakcijo« (reakcijo brez topila), se da pospešiti z dodatkom minimalne množine butan-1-ola ali toluena. Ugotovili smo namreč, da nekateri hlapni reagenti kondenzirajo v zgornjih (bolj hladnih) delih reakcijske ampule. Dodatek majhne množine butan-1-ola ali toluena je kondenzat vrnil v del ampule, kjer je potekala reakcija in tako omogočil boljši stik med reaktanti. Butan-1-ol je namreč bolj hlapen od uporabljenih maleimidov in je tudi manj viskozen, zato uspešno »spira« kondenzate maleimidov iz višje lege v ampuli, v del, kjer poteka reakcija. Ko smo uporabljali butan-1-ol kot topilo, je reakcija potekala bolj počasi, kot pod navedenimi pogoji, kar pomeni, da je uporaba butan-1-ola v večji množini manj primerna kot njegova uporaba v majhni množini (*OK4*). Poleg tega se da opisano reakcijo uspešno izvajati tudi v vodnih raztopinah ob uporabi mikrovalovnega obsevanja. Če so na izhodnih spojinah prisotne občutljive funkcionalne skupine, pa je bolj primerno izvajanje reakcije brez prisotnih topil (*OK11*).

Raziskovali smo tudi reakcije različno substituiranih 2,3:5,6-dianhidridov biciklo[2.2.2]okt-7-en-2*ekso*,3*ekso*,5*ekso*,6*ekso*-tetrakarboksilne kisline z različnimi hidrazini. Izhodne dianhidride smo v vodni raztopini pod pogoji mikrovalovnega obsevanja z visokimi izkoristki pretvorili v ustrezne pripojene *N*-aminosukcinimide. Kadar je izhodni derivat vseboval dodatno acetilno skupino, pa je reagirala tudi ta in tako se je derivat pretvoril v ustrezne hidrazone *N*-aminosukcinimidov, kot edine produkte (*OK10*).

Opisali smo tudi »one-pot« sintezo 3-benzoilamino derivatov 5- do 8-členskih cikloalka[*b*]piran-2-onov in 2*H*-piran-2-onov, izhajajoč iz primernih alkanonov, *N*,*N*-dimetilformamid dimetil acetala (DMFDMA) in hipurne kisline, v velikem prebitku acetanhidrida. Primerjali smo konvencionalno termično aktivacijo z mikrovalovno. Benzoilno zaščitno skupino na aminski skupini piran-2-onskih derivatov smo odstranili z rahlim segrevanjem v žveplovi kislini in z visokimi izkoristki pripravili ustrezne 3-aminocikloalka[*b*]piran-2-one ter 3-amino-2*H*-piran-2-one (*OK1*).

Iz ustreznih izocianatov in alkil karbazatov smo pripravili več nesimetričnih diazendikarboksamidov. Tako je adicija alkil karbazata na izocianat vodila do tvorbe 1,4-disubstituiranega semikarbazida. Oksidacijo slednjega smo izvedli z NBS/Py ali pa s CAN in je dala stabilen alkil aminokarbonildiazenkarboksilat. Kot najprimernejša pot do nesimetričnega diazendikarboksamida se je pokazala substitucija alkoksi skupine v diazenkarboksilatu s primarnim aminom kot nukleofilom. Po drugi strani pa je mogoče sintezo simetričnih diazendikarboksamidov realizirati z uporabo dveh ekvivalentov ustreznega primarnega amina. Redukcija poljubnega diazendikarboksamida z različnimi tioli je vodila do njegovega hidrazindikarboksamida. Aminokarbonildiazenkarboksamide smo pripravili podobno kot je opisano zgoraj, le da smo uporabili monosubstituirane hidrazine namesto alkil karbazatov. Serijo semikarbazidov, aminokarbonildiazenkarboksilatov, diazendikarboksamidov in hidrazindikarboksamidov smo testirali kot inhibitorje D-alanin-D-alanin ligaze (Ddl) iz *Escherichia coli*. Ddl namreč katalizira biosintezo prekurzorja esencialnega bakterijskega peptidoglikana, D-alanil-D-alanina, in zato predstavlja pomembno tarčo za razvoj novih antibakterijskih učinkovin. Najpomembnejši inhibitor Ddl je strukturni analog D-alanina in sicer D-cikloserin. Poudariti velja, da smo za 13 diazendikarboksamidov ugotovili, da so boljši inhibitorji kot D-cikloserin, kar predstavlja obetajoče izhodišče za nadaljnje raziskave (*OK2*). Rezultate te študije smo najprej pokrili s patentno prijavo (*OK59*).

Podobnim diazenom, kot so navedeni zgoraj, smo ugotavljali citotoksičnost proti naslednjim celičnim linijam levkemije: NALM-1, JURKAT, HL-60 in K-562. Več spojin je pokazalo visoko aktivnost proti dvema ali celo trem linijam levkemije (IC_{50} < 50 μM). Potrebno je povedati, da ti diazeni ne učinkujejo na zdrave celice (‚Con-A-stimulated PBMC', ‚resting PBMC', 3T3 fibroblasti) (*OK35*).

Izoniazid (INH) in pirazinkarboksamid (PZA) sta v kombinaciji z drugimi zdravili široko uporabni »zdravili prve linije« (first-line drugs) za zdravljenje tuberkuloze. V iskanju bolj učinkovitih zdravil proti TBC smo načrtovali in sintetizirali nove derivate, ki imajo v molekuli izoniazid, pirazinkarboksamid in druge fragmente, povezane s CH skupino. To novo vrsto molekul lahko obravnavamo kot »dvojno aktivno«, ki lahko služi kot »prozdravilo« s podaljšanim sproščanjem. Komponente vključene v molekulo lahko omogočajo sinergijo. V skladu s tem načrtom smo INH obdelovali z *N*,*N*-dimetilformamid dimetil acetalom, pri čemer je nastal *N*'-4-izonikotinoil-*N*,*N*-dimetilhidrazonoformamid kot potencialna startna spojina za pripravo drugih INH derivatov. Na žalost se je izkazalo, da je dimetilaminska skupina preslaba izstopajoča skupina za naše potrebe. Zato smo iz INH pripravili hidrazon z uporabo dietoksimetil acetata. Nastali etoksimetilenhidrazon je namreč znan kot dober vir C1 fragmenta, ki ga lahko uporabimo za tvorbo C–N ali pa C–C vezi. Tako smo etoksimetilenhidrazon s primarnimi in sekundarnimi amini pretvorili v ustrezne formamidrazone. Sledila je zamenjava etoksi skupine s primernimi dušikovimi nukleofili (morfolin, 2-aminometilpiridin, benzilamin, *para*-aminosalicilna kislina (PAS), ciprofloksacin (CPF) in INH), ki je dala produkte formamidinskega tipa, kjer sta bila INH in izbrani dušikov nukleofil povezana s CH skupino. Produkta z vključenim PZA ali pa CPF sta bila deležna posebne pozornosti, ker ju lahko obravnavamo kot prozdravili, saj imata dve običajni učinkovini povezani s CH fragmentom (INH-PAS, INH-CPF).

Tudi produkt hidrazona z INH združuje v molekuli dve, sicer identični enoti (INH-INH). Podoben pristop smo uporabili za funkcionalizacijo pirazinkarboksamidne molekule. Tako smo z obdelavo aktiviranega pirazinskega derivata, *N*-dimetilaminometilen)pirazin-2-karboksamida, s CPF dobili 1-ciklopropil-6-fluoro-4-okso-7-{[4-(pirazin-2-ilkarbonil)iminometil]pipera zin-1-il}-1,4-dihidrokinolin-3-karboksilino kislino (PZA-CPF), medtem, ko je reakcija s PSA vodila do tvorbe 4-(2-pirazinkarboniliminometil)aminosalicilne kisline (PZA-PAS). Največjo antimikobakterijsko aktivnost proti *Mycobacterium tuberculosis* $H_{37}R_v$ smo ugotovili za PZA-INH, PZA-PAS, INH-PAS in INH-INH (MIC vrednosti: 0.1−0.78 μg/mL) (*OK3*).

Raziskali smo ne prav pogosto opisane elektrofilne aromatske ipso-substitucije acilnih skupin s protonom z uporabo različnih mineralnih kislin. Ugotovili smo, da takšne zamenjave potečejo tako v brezvodnem mediju, kot tudi v prisotnosti vode. Potreben pogoj in s tem omejenost pri izbiri substratov je prisotnost močno elektron-donorske skupine na aromatskem jedru. V doslej znanih primerih je bila takšna pretvorba mogoča le, če je bila acilna skupina sterično ovirana s substituentom na *orto* položajih. Naše ugotovitve so dopolnilo k znanju na področju elektrofilnih aromatskih substitucij, ki spadajo med osnovne metode sintezne kemije (*OK26*).

Zaradi izrednega zanimanja strokovne javnosti za uporabo 2-(1-{6-[(2-[^{18}F]fluoroetil)(metil) amino]-2-naftil}etiliden)malononitrila ([^{18}F]FDDNP) v raziskavah nevrodegenerativnih bolezni, pri katerih se v možganih izločajo proteinski agregati, smo razvili avtomatizirano sintezo. Sinteza je hitra in zanesljiva in omogoča pripravo velikih množin (>150 mCi) [^{18}F]FDDNP za uporabo pri glodalcih in ljudeh (*OK22*).

β-Ketoamidi in β-ketoestri so skupina spojin, ki predstavljajo uporabne izhodne spojine v organski sintezni kemiji. Razvili smo uspešen postopek za sintezo zgoraj omenjenih tipov spojin, ki temelji na uporabi 2,2-difluoro-4-alkoksi-1,3,2-dioksaborininov kot izhodnih spojin (*OK30*).

Opisali smo enostavno sintezno metodo za pripravo serije 1,4-disubstituiranih 5-hidroksi-1*H*-pirazolov iz 2-fenil-4-hidroksimetilidenoksazol-5(4*H*)-ona in različnih fenilhidrazinov. Prvi del te metode je *in situ* priprava etil formilhipurata, kar dosežemo z reakcijo oksazolona z etanolom. Nato izvedemo reakcijo estra z izbranim fenilhidrazinom, ki vodi do tvorbe ustreznega hidrazona. Zadnja stopnja pa je ciklizacija hidrazona v *N*-(1-fenil-5-hidroksi-1*H*-pirazol-4-il)benzamidni derivat v prisotnosti NaOH (*OK36*).

Z NMR, MS in rentgensko difrakcijsko analizo smo določili strukturi dveh stranskih produktov s spiro[2*H*-indol]-3(1*H*)-onskim skeletom, ki sta spremljala premestitev 1-fenil-3-hidroksi-3-metilkinolin-2,4(1*H*,3*H*)-diona v 1-fenil-2-hidroksi-2-metil-1,2-dihidro-3*H*-indol-3-on. Čeprav sta v omenjeni reakciji stranska produkta nastala v majhnih množinah, je spiro[2*H*-indol]-3(1*H*)-onski strukturni motiv pomemben, saj je sestavni del nekaterih naravnih produktov, biološko aktivnih molekul in spojin s fotokromnimi lastnostmi (*OK21*).

DRUGI RELEVANTNI DOSEŽKI

Opisali smo uporabo alkenske metateze za pripravo uporabnih kemikalij in supramolekularnih sistemov (*OK49*).

Del raziskav članov programske skupine poteka tudi v okviru raziskovalnega projekta *Od multifunkcionalnih gradnikov do biološko aktivnih spojin*, delno pa smo bili vključeni tudi v raziskave za industrijo.

Člani programske skupine smo opravili tudi več predavanj (plenarnih, vabljenih idr.) na mednarodnih konferencah, univerzah ali inštitutih.

Prof. M. Kočevar je postal Nacionalni predstavnik v odboru (komiteju) Organic and Biomolecular Chemistry Division (III) IUPAC (za obdobje 2008−2009).

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

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

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

Within the framework of the research programme COST D24/007 we have been developing novel methods for the synthesis and hydrogenation of sterically constrained heteropolycyclic derivatives of bicyclo[2.2.2]octene. Double Diels−Alder reaction of a series of 2*H*-pyran-2-one derivatives and *N*-substituted maleimides, in which the corresponding bicyclo[2.2.2]octenes are formed, was carried out in green conditions in water and under microwave irradiation. The products thus obtained were used for the investigation of heterogeneous hydrogenation by the application of ionic immobilized complexes of Rh on LDH (layered double hydroxide) surface. The catalyst was prepared from $[Rh(cod)Cl]_2$ (as a source of rhodium ions), hydroxides of Zn_3AlCl or Co_2FeCO_3 (as LDH) and two water-soluble ligands: trisodium salt of triphenylphosphine-3,3′,3′′-trisulfonat (TPPTS) or lithium triphenylphosphine-3,3′,3′′-tricarbonate (*m*-TPPTC). The catalysts thus prepared can be regenerated and re-used without significant loss of selectivity. The emphasis of this research work was optimization of the catalyst Rh/TPPTS/LDH for the hydrogenation of our substrates and hydrogenation under optimized conditions. A research group from the University in Salamanca, Spain participated in this study. The catalyst was characterized by applying several techniques: chemical composition of the catalysts was determined using ICP atomic emission spectrometry. N_2 adsorption-desorption isotherms of the LDH support were measured at −196 °C with a Micromeritics ASAP 2020. We also used powder X-ray diffraction analysis, etc. Our results have shown that sterically constrained substrates are inert toward the hydrogenation applying conventional catalysts, but they can be hydrogenated using ionic immobilized complexes Rh-ligand on LDH (*OK17*).

The Diels−Alder reaction of *2H*-pyran-2-ones with a series of *N*-substituted maleimides yielding derivatives of bicyclo[2.2.2]octene, which was carried out under microwave irradiation condition as a neat reaction (reaction in the absence of solvent), can be accelerated by the addition of a minimal amount of butan-1-ol or toluene. We have shown that some volatile reagents condense in the upper (cooler) parts of the reaction ampoule. By adding a small amount of butan-1-ol or toluene the condensate was washed down to the part of the ampoule, where the reaction took place, thus providing a better contact between the reagents. Butan-1-ol is more volatile than the maleimides used and also less viscous; therefore it is successful in washing

down condensates of maleimides to the lower part of the reaction ampoule. When we used butan-1-ol as a solvent the reaction ran more slowly than under above-mentioned conditions; this means that the application of butan-1-ol in larger amounts (as a solvent) is less appropriate than its use with a smaller amount (*OK4*). The above reactions can also be carried out in aqueous solutions and under microwave irradiation conditions. If sensitive functional groups are present as a part of the starting compounds, it is more convenient to use reaction condition in the absence of any solvent (*OK11*).

The reaction of variously substituted bicyclo[2.2.2]oct-7-ene-2*exo*,3*exo*,5*exo*,6*exo*-tetracarboxylic acid 2,3:5,6-dianhydrides with a set of hydrazines was investigated. The starting dianhydrides were transformed into an aqueous solution under microwave irradiation conditions to the corresponding fused *N*-aminosuccinimides with high yields. The starting derivative possessing an additional acetyl moiety reacted also at this additional group to give the corresponding hydrazono derivatives of *N*-aminosuccinimides as the sole products (*OK10*).

A one-pot synthesis of 3-benzoylamino derivatives of 5- to 8-membered cycloalka[*b*]pyran-2-ones and 2*H*-pyran-2-ones, starting from the appropriate alkanones, *N*,*N*-dimethylformamide dimethyl acetal (DMFDMA) and hippuric acid in the presence of a large excess of acetic anhydride was also described. A comparison of the conventional thermal activation with microwave activation was investigated. The benzoyl protective group on the amino moiety of pyran-2-one derivatives was successfully removed by gentle heating in sulfuric acid resulting in the formation of the corresponding 3-aminocycloalka[*b*]pyran-2-ones and 3-amino-2*H*-pyran-2-ones in high yield (*OK1*).

Several unsymmetrical diazenedicarboxamides were prepared starting from the corresponding isocyanates and alkyl carbazates. Thus, an addition of alkyl hydrazinecarboxylate to the isocyanate resulted in the formation of 1,4-disubstituted semicarbazide. Oxidation of the latter was then performed with either NBS/pyridine or CAN to give a stable alkyl aminocarbonyldiazenecarboxylate. The most convenient route to unsymmetrical diazenedicarboxamides turned out to be the substitution of an alkoxy group in the diazenecarboxylate employing a primary amine as a nucleophile. On the other hand, the synthesis of symmetrical diazenedicarboxamides involved a treatment of a commercially available dialkyl diazenedicarboxylates with two equivalents of an appropriate primary amine. A reduction of any diazenedicarboxamide with various thiols led to the formation of its hydrazinedicarboxamide. Alkylaminocarbonyldiazenecarboxamides were obtained similarly as decribed for unsymmetrical diazenedicarboxamides using monosubstituted hydrazines in the place of alkyl carbazates. A series of semicarbazides, aminocarbonyldiazenecarboxylates, diazenedicarboxamides, and hydrazinedicarboxamides was screened for inhibition of D-Alanine-D-alanine ligase (Ddl) from *Escherichia coli*. Ddl catalyzes the biosynthesis of an essential bacterial peptidoglycan precursor D-alanyl-D-alanine and it represents an important target for the development of new antibacterial drugs. So far, the most important inhibitor of Ddl is a structural analog of D-alanine, the antitubercular agent D-cycloserine. It should be noted that 13 diazenedicarboxamides are better inhibitors than D-cycloserine and some of them also possess antibacterial activity, which makes them a promising starting point for further development (*OK2*). The results from this study were first covered by a patent application (*OK59*).

Diazenes, which belong to the same categories as those mentioned above, were evaluated for their cytotoxicity against the following human leukemic cell lines: NALM-1, JURKAT, HL-60, and K-562. Several compounds possessed high efficacy to two or three leukemic cell lines (IC_{50} < 50 μM). In addition, they did not affect normal cells (Con-A-stimulated PBMC, resting PBMC, 3T3 fibroblasts) (*OK35*).

Isoniazid (INH) and pyrazinecarboxamide (PZA) are widely applied as first-line drugs for the treatment of tuberculosis, usually in combination with other drugs. In the quest for biologically more potent anti-tuberculosis compounds we have designed and synthesized new derivatives that contain isoniazid, pyrazinamide, and some other moieties linked by the CH group. This new type of molecule can be regarded as a 'double active' molecule that can play the role of a prodrug with a prolonged liberation. In addition, the components involved in it may act synergetically. Following this plan, we first treated INH with *N*,*N*-dimethylformamide dimethyl acetal to obtain *N*'-4-isonicotinoyl-*N*,*N*-dimethylhydrazonoformamide as a starting compound to obtain other INH derivatives. Unfortunately, the dimethylamino group turned out to be a poor leaving group for our purposes. Therefore, we prepared hydrazone from the INH by employing diethoxymethyl acetate as a good synthon of the CHOEt fragment. Namely, this hydrazone is known as a good source of the C1 fragment that can serve for the formation of either a C–N or a C–C bond. Thus, the treatment of ethoxymethylene hydrazone with primary or secondary amines resulted in the formation of the corresponding formamidrazones. In the present study, the ethoxy group of the above hydrazone was substituted with nitrogen nucleophiles (morpholine, 2-aminomethylpyridine, benzylamine, *p*-aminosalicylic acid (PAS), ciprofloxacin (CPF), and INH) to afford the formamidine-like products, where the INH and the nitrogen nucleophile are connected with the CH group. The products obtained employing PAS and CPF were given special attention. This is because they can be considered as prodrugs that contain two conventional drugs connected by a CH fragment (INH-PAS, INH-CPF). In addition, the product from hydrazone and INH binds two identical fragments, that is, two INH molecules (INH-INH). A similar approach has been used to functionalize the pyrazinamide molecule. The treatment of an activated pyrazine derivative, *N*-(dimethylaminomethylene)pyrazine-2-carboxamide, with CPF gave the desired 1-cyclopropyl-6-fluoro-4-oxo-7-{[4-(pyrazin-2-ylcarbonyl)iminomethyl]piperazin-1-yl}-1,4-dihydroquinoline-3-carboxylic acid (PZA-CPF), while reaction with PAS resulted in the formation of 4-(2-pyrazinecarbonyliminomethyl) aminosalicylic acid (PZA-PAS). The highest antimycobacterial activities against *Mycobacterium tuberculosis* $H_{37}R_v$ were found for PZA-INH, PZA-PAS, INH-PAS, and INH-INH (MIC values: 0.1−0.78 μg/mL) (*OK3*).

We have also investigated less frequently described electrophilic aromatic ipso-substitutions of acyl groups by hydrogen, using various mineral acids. We discovered that such transformations take place with strong mineral acids in aqueous or anhydrous media. The requirement for a successful reaction is the presence of a strong electron-donating group in a conjugated position. In the examples reported so far, such transfromations are possible only if the acyl group is sterically hindered by substituents in *ortho* positions. Our findings have contributed to the knowledge on electrophylic aromatic substitutions and represent the basic methods of organic synthetic chemistry (*OK26*).

Prompted by extraordinary interest in utilization of 2-(1-{6-[(2-[^{18}F]fluoroethyl)(methyl)amino]-2-naphthyl}ethylidene)malononitrile ([^{18}F]FDDNP) in PET research of neurodegenerative disorders in which protein aggregates accumulate in the central nervous system, we developed a high-yield automated radiosynthesis. The method is rapid, reliable, and suitable for preparing large amounts (>150 mCi) of [^{18}F]FDDNP for rodent and human studies (*OK22*).

4-Alkoxy substituted 1,3,2-dioxaborinines, readily available from β-keto esters, undergo substitution reactions under mild reaction conditions with primary and secondary amines, producing 4-alkylamino analogues. Reactions of 1,3,2-dioxaborinines with substituted phenylhydrazines gave the corresponding hydrazones, or pyrazolones, and 5-alkoxy-1*H*-pyrazoles as a mixture of products (*OK30*).

We have described a simple synthetic method for the preparation of a series of 1,4-disubstituted-5-hydroxy-1*H*-pyrazoles from 4-hydroxymethylidene-2-phenyloxazol-5(4*H*)-one and various phenylhydrazines. The first part of the method is *in situ* preparation of ethyl formylhippurate, which is achieved by the reaction of the oxazolone with ethanol. Therefore, the treatment of the ester with a chosen phenylhydrazine leads to the formation of a corresponding hydrazone derivative. The last step is the cyclization of the hydrazone in the presence of NaOH into *N*-(5-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)benzamide derivative (*OK36*).

Molecular structures of two by-products possessing spiro[2*H*-indol]-3(1*H*)-one skeletons, which accompanied the rearrangement of 3-hydroxy-3-methyl-1-phenylquinoline-2,4(1*H*,3*H*)-dione into 2-hydroxy-2-methyl-1-phenyl-1,2-dihydro-3*H*-indol-3-one, have been elucidated by NMR, MS, and X-ray diffraction. Even though the by-products in the above mentioned reaction are formed in minute amounts, the spiro[2*H*-indol]-3(1*H*)-one structural motif is important as it has been found in some natural products, and is a constituent element of some biologically active molecules and compounds with photochromic properties (*OK21*).

OTHER RELEVANT ACHIEVEMENTS

We have described some recent applications of alkene metathesis reaction for fine chemicals and supramolecular system synthesis (*OK49*).

Some members of the research programme group were partially engaged in the research project *From multifunctional building blocks to biologically active compounds*. We were also partially involved in some projects with industry.

Several lectures (plenary, invited, etc.) were delivered at international conferences, universities and institutes.

Prof. M. Kočevar has been appointed as a National Representative of IUPAC Organic and Biomolecular Chemistry Division (III) Committee for the period 2008−2009.

KEMIJSKO INŽENIRSTVO
CHEMICAL ENGINEERING

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P2–0191

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POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Cilji programa so opredeljeni po delitvi vsebine programa na osrednje teme, ki so: *modeliranje in procesno inženirstvo, reologija in aplikacije, polimerno inženirstvo in tehnologija, biokemijsko inženirstvo in biotehnologija* ter *okoljsko inženirstvo in aplikacije.*

MODELIRANJE IN PROCESNO INŽENIRSTVO

Obravnavali smo proces retencije koloidnih delcev alkilketen dimera na celuloznih vlaknih, ki poteka med pripravo papirne mase v proizvodnji papirja. Alkilketen dimer (AKD) v papirju nastopa v vlogi klejiva – uravnava prodiranje tekočine v papir oziroma papirju zagotovlja določeno stopnjo hidrofobnosti. Za napoved retencije koloidnih delcev AKD na celulozna vlakna smo razvili matematični model na osnovi opisa trkov med delci.

Že zbrana podatkovna baza deleža plina v raztopinah CMC in ksantana, posneta na koloni s perforirano ploščo, je bila analizirana z v literaturi uveljavljenima modeloma (angl.: *drift-flux model* in angl.: *slip velocity model*) in konfrontirana z razvitima korelacijama za napoved deleža plina. Kontinuiteta študija hidrodinamskih parametrov klasične kolone z mehurčki s sintrano ploščo kot distributorjem je bila zagotovljena z izvedbo načrtovanih dodatnih eksperimentov z ksantanovimi raztopinami srednjega razreda, dokumentirana s kvalitativno sledilno tehniko.

Nadaljevali smo z raziskavami nanofiltracije v sistemih z organskimi topili z namenom koncentriranja aktivnih farmacevtskih učinkovin. Za izbrani sistem učinkovine in topila smo primerjali koncentriranje z nanofiltracijo in uparjanjem.

REOLOGIJA IN APLIKACIJE

Vpliv hidratiziranega apna (H-apna) na lastnosti bitumenske malte (zmesi polnila in bitumna) in lastnosti bitumenskih veziv smo preverili s standardnimi testi in reološkimi meritvami. Uporabljeni so bili bitumni B50/70 (Mantova) in PmB II (Villabit 65), ki se pri nas uporabljajo za proizvodnjo asfaltnih zmesi za obrabne in obrabno zaporne plasti. V zmeseh smo del polnila nadomestili s H-apnom. Delež H-apna v polnilu je znašal med 0 in 20 ut%. Vzorci so bili preiskani, pred in po temperaturnem staranju, ter po ekstrakciji iz bitumenske malte.

Reološke raziskave za plaz Slano Blato pri Ajdovščini: V zadnjem desetletju so bili prvi večji premiki na plazu l. 2000. Največji izmerjeni pomiki splazele mase so bili 60–100 m/dan. Leta

2004 so se izvajale geotehnične raziskave z namenom pridobitve podatkov sanacije plazu. V sklopu teh raziskav so bile izvedene obsežne reološke raziskave. Analiza vseh podatkov je potekala tudi v zadnjem letu.

Določanje hitrostnoega polja v nenewtonski kapljevini znotraj mešalne posode s šestlopatičnim mešalom z ravnimi lopaticami: Viskoznost je bila med mešanjem določena s pomočjo merjenja navora pri različnih hitrostih mešala ter primerjave z reološko dobljeno strižno odvisno viskoznostjo.

Analiza vnosa moči pri mešanju in dispergiranju zraka v ne-newtonski tekočini z Rushtonovo turbino v standardni cilindrični mešalni posodi: Uporabili smo vodne raztopine karboksi metil celuloze (CMC) s koncentracijo $w = 0.5$ % and $w = 1$ % in stisnjen zrak, ki smo ga vpihavali z različnimi pretoki. Izmerjeno navidezno viskoznost raztopin smo uporabili za določitev zveze med strižno hitrostjo in številom obratov mešala, pri čemer smo uporabili pravilo Metzner-Otto. Tako smo izračunali število moči v odvisnosti od Reynoldsovega števila. Primerjava eksperimentalno določene porabe moči pri mešanju enofaznega sistema za ne-newtonske tekočine se je ujemala z rezultati iz literature. Namen dela je poiskati vpliv dispergiranega zraka na porabo moči pri procesu mešanja v dvofaznih sistemih tekočina-plin.

POLIMERNO INŽENIRSTVO IN TEHNOLOGIJA

Razvoj na področju polimernega inženirstva in tehnologije zahteva multidisciplinarne temeljne in aplikativne raziskave, ki vključujejo sintezo in karakterizacijo polimerov, polimerno inženirstvo, načrtovanje lastnosti polimernega materiala in načrtovanje tehnologije za proizvodnjo produkta. Cilji v okviru programa so bili preučiti in matematično modelirati kinetiko zamreževanja izbranih elastomernih sistemov ter prenos toplote med zamreževanjem, eksperimentalno določiti in na osnovi razvitega modela napovedovati viskoelastično obnašanje elastomernih materialov v širokem temperaturno-frekvenčnem območju, pripraviti in okarakterizirati elastomerne nanokompozitne materiale, razviti testno metodo za določevanje abrazijske odpornosti zobatega pogonskega jermena, preučiti in modelirati kinetiko sinteze fenol-formaldehidnih smol in melaminsko-formaldehidnih smol, osvojiti tehnologijo priprave melaminskih pen, optimizirati sintezo in lastnosti mikrosfernih, na pritisk občutljivih akrilatnih lepil, preučiti sintezo enokomponentnih poliuretanskih lepil, razviti lepilo ter optimizirati njegove lastnosti in razviti »in-line« merilni sistem za novo aparaturo za ekspanzijsko injekcijsko stiskanje polimernih talin.

BIOKEMIJSKO INŽENIRSTVO IN BIOTEHNOLOGIJA

Na osnovi dosedanjih raziskav vpliva bioprocesnih parametrov na morfologijo glive *Rhizopus nigricans* in pa določitve kinetičnih parametrov procesa biotransformacije progesterona v prisotnosti β-ciklodekstrina smo postavili kontinuirno biotransformacijo steroidov v laboratorijskem bioreaktorju v prisotnosti omenjenega solubilizacijskega sredstva s peleti različnih velikosti. Da bi uspeli postaviti integriran proces biotransformacije progesterona, smo izvedli in modelirali tudi kontinuirno ekstrakcijo produktov obravnavane biotransformacije v mikroreaktorju, ki omogoča izredno učinkovit prenos snovi in majhno porabo kemikalij.

Potrebe po hitrem odkrivanju in proučevanju mehanizmov novih sinteznih poti, (bio)katalizatorjev in ustreznih reaktantov za pridobivanje novih produktov so vodile v razvoj sistemov, ki ne zavzemajo veliko prostora, so enostavni za uporabo, porabijo malo reagentov in dajejo malo odpadnega materiala, hkrati pa so sprejemljivi za okolje in zadržujejo

vse pozitivne lastnosti običajnih eksperimentalnih tehnik. Eno od obetavnih alternativ, ki izpolnjuje vse navedene zahteve, predstavljajo reaktorji submilimetrskih dimenzij – mikroreaktorji. Njihova uporaba v (bio)kemijskih procesih v zadnjih letih zelo narašča, saj omogočajo hitrejši prenos rezultatov razvoja v proizvodnjo, zgodnejši začetek proizvodnje z manjšimi sredstvi, enostavnejše povečanje obsega proizvodnje (t.i. ”numbering-up” namesto ”scale-up”), manjšo velikost tovarne, manjše stroške za material in energijo in bolj prilagodljiv odgovor na zahteve trga. Vendar pa je objavljenih le malo študij ter patentov o biokataliziranih procesih v mikroreaktorjih. Namen naših raziskav je implementacija mikroreaktorske tehnologije v biokatalitske procese in opredelitev osnovnih transportnih pojavov ter toka tekočin v mikrokanalih s pomočjo sodobnega modeliranja. Poleg tega nameravamo razviti okolju prijazne mikroreaktorske tehnologije, tudi z uporabo ionskih kapljevin, ki jih zaradi številnih ugodnih lastnosti (nehlapnost, odlična toplotna stabilnost, visoka sposobnost raztapljanja organskih snovi, negorljivost, visoka prevodnost) imenujemo tudi »zelena topila«. Njihova uporaba je zaradi visoke cene v industrijskem merilu zelo omejena, zato je postavitev procesa v mikroreaktorskem sistemu lahko obetavna alternativa.

Farmacevtske učinkovine glive *Grifola frondosa*: V sklopu projekta so raziskave potekale v treh smereh : (1) submerzna kultivacija v mešalnem bioreaktorju v tekočem gojišču, kjer smo se osredotočili na selekcijo in optimizacijo gojišč za produkcijo biomase ter farmacevtsko aktivnih snovi ter možnosti izkoriščanja industrijskih odpadkov; (2) kontrolirano gojenje v bioreaktorju za sterilizirana trdna gojišča (solid-state) iz agroživilske in lesne industrije; (3) gojenje gob v eksperimentalni farmi gob. Cilj tega dela je selekcija in optimizacija gojišč za tvorbo biomase, farmacevtsko aktivnih spojin ter procesiranje, vnovična uporaba težavnih odpadkov in pridelava zadostnih količin gobje biomase za nadaljnje testiranje. Ob tem smo študirali vpliv različnih okoljskih parametrov na tvorbo samih plodišč ter izbrali in optimizirali najboljše substrate.

Nadaljevali smo raziskave gojenja aktivne glivine biomase s postopkom kultivacije na trdnem gojišču na osnovi koruzne slame, koruznih storžev, droblja in žagovine. Paralelno s tem so tekle osnovne raziskave produkcije aktivne glivine biomase v smislu gojenja gob na eksperimentalni farmi.

V sklopu raziskav biokemijskega inženirstva v vinarstvu smo študirali vpliv temperaturnega šoka na vcepek vinskih kvasovk in njegov učinek na metabolizem *Saccharomyces cerevisiae* v alkoholni fermentaciji vinskega mošta in pri tem razvili nov originalni tehnološki postopek, ki omogoča produkcijo visokih dobitkov glicerola v vinih. Preučili smo pomen tehnoloških parametrov kot so vpliv temperature, kisika in mešanja na nastajanje vina.

OKOLJSKO INŽENIRSTVO IN APLIKACIJE

Nadaljevali smo z raziskavami na področju bioremediacije. Proučevali smo encimske aktivnosti MnP in Lac pri glivi *Ceriporiopsis subvermisporas* v mediju po Kirku, ki smo mu dodali različne vire sladkorjev, dušik v obliki amonijevega tartrata in jih gojili v imobilizirani obliki na različnih vrstah lesa. Z nastalimi encimi smo proučevali razgradnjo izbranih sintetičnih barvil.

OSREDNJE TEME PROGRAMA

Modeliranje in procesno inženirstvo:

- Aplikativne, procesno inženirske raziskave proizvodov na osnovi fosfornih spojin prve generacije in produktno inženirske raziskave nove generacije proizvodov
- Sinteza kelatov za agrokemijske namene
- Študij adsorpcije biocidov v praškastih formulacijah
- Membransko oplaščanje umetnih gnojil s podaljšanim delovanjem
- Študij procesa retencije koloidnih delcev alkilketen dimera na celuloznih vlaknih
- Študij delovanja kolone z mehurčki (perforirana plošča kot plinski distributor) v prisotnosti ne-newtonskega medija
- Membranske separacije – raziskave nanofiltracije v sistemih z organskimi topili

Reologija in aplikacije:

- Vpliv hidratiziranega apna (H-apna) na lastnosti bitumenske malte
- Reološke raziskave za plaz Slano Blato pri Ajdovščini
- Določanje hitrostnega polja v ne-newtonski kapljevini znotraj mešalne posode s šestlopatičnim mešalom z ravnimi lopaticami
- Analiza vnosa moči pri mešanju in dispergiranju zraka v nenewtonski tekočini z Rushtonovo turbino v standardni cilindrični mešalni posodi

Polimerno inženirstvo in tehnologija:

- Študij kinetike vulkanizacije različnih gumenih zmesi in modeliranje
- Študij prenosa toplote med vulkanizacijo različnih gumenih zmesi in modeliranje
- Sinteza, priprava in karakterizacija nanokompozitnih materialov
- Testiranje mehanskih lastnosti gume in gumenih kompozitov
- Sinteza, karakterizacija in optimizacija procesa sinteze fenol-formeldehidnih smol, sečninsko-formaldehidnih smol, melaminsko-formaldehidnih smol, fenol-sečninsko-formaldehidnih smol, melamin-sečninsko formaldehidnih smol
- Raziskave na področju tehnologije priprave melaminskih pen
- Sinteza, karakterizacija in optimizacija procesa sinteze akrilatnih lepil
- Sinteza, karakterizacija in optimizacija procesa sinteze enokomponentnih poliuretanskih lepil
- Raziskave na področju ekspanzijskega injekcijskega stiskanja

Biokemijsko inženirstvo in biotehnologija:

- Kontinuirni proces biotransformacije steroidov
- Ekstrakcija steroidov v mikroreaktorju
- Biokatalitske reakcije v mikroreaktorju
- Študij encimsko katalizirane sinteze izoamil acetata
- Submerzna biosinteza ekstra in intracelularnih učinkovin
- Kultivacija glivine biomase ekstra in intracelularnih učinkovin na trdnem gojišču
- Gojenje gliv na odpadkih lesno predelovalne industrije na eksperimentalni farmi gob
- Izolacija in purifikacija glivinih polisaharidov
- Testiranje aktivnosti indukcije citokinov na človeških celičnih linijah

– Postopki za zvišanje produkcije glicerola
– Uporaba termošoka na vcepku kvasovk *Saharomyces cerevisiae*

Okoljsko inženirstvo in aplikacije:
– Raziskave na področju bioremediacije

ZNANSTVENI DOSEŽKI

MODELIRANJE IN PROCESNO INŽENIRSTVO

Študij procesa retencije koloidnih delcev alkilketen dimera na celuloznih vlaknih: Obravnavali smo proces retencije koloidnih delcev alkilketen dimera na celuloznih vlaknih, ki poteka med pripravo papirne mase v proizvodnji papirja. Alkilketen dimer (AKD) v papirju nastopa v vlogi klejiva – uravnava prodiranje tekočine v papir oziroma papirju zagotovlja določeno stopnjo hidrofobnosti. Za napoved retencije koloidnih delcev AKD na celulozna vlakna smo razvili matematični model na osnovi opisa trkov med delci. Uporabili smo modificirano Langmuirjevo enačbo, ki opisuje process retencije v odvisnosti od zasedenosti površine in definirali hitrostne konstante. Napovedi vrednosti ravnotežnih retencij na osnovi modela se dobro ujemajo z eksperimentalnimi podatki. Analiza površinske napetosti sistema je potrdila, da obseg in učinkovitost trkov delcev AKD z celuloznimi vlakni ključno vpliva na uspešno retencijo (*KIŽ5*).

Študij delovanja kolone z mehurčki (perforirana plošča kot plinski distributor) v prisotnosti ne-newtonskega medija: Rezultati zaključenega študija delovanja kolone z mehurčki (perforirana plošča kot plinski distributor) v prisotnosti nenewtonskega medija so pokazali razliko v obnašanju vodnih raztopin karboksi metil celuloze in vodnih raztopin ksantana, predvsem v pogojih dvofaznega toka. Raztopine CMC so pokazale potenčno odvisnost deleža plina od efektivne viskoznosti tekočine, kar je omogočilo razvoj korelacije za napoved deleža plina v odvisnosti od obratovalnih pogojev. Raztopine ksantana izkazujejo lastnosti šibkih gelov, tako da je vpliv efektivne viskoznosti tekočine na performanco kolone kompleksnejši, kar stimulira nadaljnje raziskave na tem področju (*KIŽ18*).

Membranske separacije: Primerjava uparjanja in nanofiltracije pri koncentriranju aktivne farmacevtske učinkovine je pokazala, da je koncentriranje z nanofiltracijo bistveno cenejše od uparjanja.

REOLOGIJA IN APLIKACIJE

Vpliv H-apna na lastnosti bitumenske malte: Vpliv H-apna na lastnosti bitumenske malte je odvisen od izbranega bitumna. Neodvisno od tipa bitumna H-apno v zmeseh bitumna in polnila najbolj vpliva na viskoznost zmesi. Ugotovili smo, da zmes bitumna s polnilom, ki vsebuje H-apno utrdi, stopnja utrditve pa je odvisna od vsebnosti H-apna in tipa bitumna. Lastnosti zmesi pri nizkih temperaturah se do določene vsebnosti H-apna ne spreminjajo, pri višjih vsebnostih pa se poslabšajo. H-apno zavira proces oksidacije, učinkovitost je večja pri polimerno modificiranemu bitumnu. Meritve ekstrahiranih vzorcev kažejo, da ni vpliva prisotnosti H-apna na lastnosti izbranih bitumnov (*KIŽ 32*).

Reološke raziskave za plaz Slano Blato pri Ajdovščini: Stabilnostne analize plazenja zemeljskega plazu so bile izvedene z Burghersovim elasto-plastičnim modelom. Model pri izračunu upošteva geomehanske karakteristike in reološke lastnosti splazele mase. Rezultati analiz so pokazali dobro ujemanje modela z dejansko dinamiko plazenja zemeljskega plazu (*KIŽ7*).

Določanje hitrostnega polja v ne-newtonski kapljevini znotraj mešalne posode s šestlopatičnim mešalom z ravnimi lopaticami: Hitrostno polje je bilo določeno s pomočjo LDA meritev na dvanajstih merilnih mestih znotraj mešalne posode. Meritve so pokazale, da sta aksilna in radialna komponenta hitrosti na vseh merilnih mestih zanemarljivi. Rezultati so pokazali periodično naravo obodne komponente hitrosti, kar je bilo potrjeno tudi z računalniško podprto vizualizacijo (KIŽ19).

Analiza vnosa moči pri mešanju in dispergiranju zraka v ne-newtonski tekočini z Rushtonovo turbino v standardni cilindrični mešalni posodi: Ko dispergiramo zrak v tekočini, katere viskoznost strižno odvisno upada, opazimo zmanjšanje porabe moči, še posebno pri višjem številu obratov mešala in pri večjih pretokih zraka. Zmanjšanje vnosa moči je večje pri raztopinah CMC s koncentracijo w = 0.5 %, kot pri tistih s koncentracijo CMC w = 1 %. Moč mešanja je bila neodvisna od hitrosti pretoka zraka pri majhnih Reynoldsovih številih. Primerjava merjenih vrednosti disperzije zraka z rezultati korelacij iz literature potrjuje splošne trende zmanševanja porabe moči na mešalu (*KIŽ4*).

POLIMERNO INŽENIRSTVO IN TEHNOLOGIJA

Kinetika vulkanizacije zmesi elastomerov: Kot referenco smo si izbrali zmes butadienskega kavčuka (BR) in naravnega kavčuka (NR). Kinetične parametre vulkanizacijskih reakcij za zmesi NR in BR smo pridobili z regresijsko analizo ob uporabi osnovanega kinetičnega modela ter na osnovi eksperimentalnih podatkov, pridobljenih z diferenčno dinamično kalorimetrijo in dinamično mehansko analizo. Zaradi temperaturne odvisnosti vseh kinetičnih parametrov smo predpostavili, da lahko to odvisnost popišemo z Arrheniusovo zvezo. Predeksponentne koeficiente in aktivacijske energije vseh parametrov smo tako izračunali iz te zveze. Uporabljen kinetični model se je dobro ujemal z eksperimentalnimi podatki, dobljenimi pri izotermnih pogojih meritev z diferenčno dinamično kalorimetrijo in dinamično mehansko analizo. Iz preučitve obnašanja prenosa toplote v začetni fazi vulkanizacije ter temperaturno odvisnih kinetičnih konstant ključnih reakcij zamreževanja smo ugotovili, da je največja zakasnitev vulkanizacije dosežena, če je delež polibutadiena v zmesi okrog 50 utežnih odstotkov. Pri tej sestavi zmesi je dosežena tudi ustrezno visoka hitrost reakcij zamreženja in dovolj nizka hitrost reakcij reverzije (*POT3*).

Prenos toplote v elastomerih: Prenos toplote igra pomembno vlogo v številnih procesih predelave elastomerov ter je celo odločujočega pomena pri nekaterih različicah procesa vulkanizacije, čeprav je redko obravnavan enakovredno kot sama kinetika zamreževanja. S tem namenom smo študirali prenos toplote v različnih elastomerih na pilotni stiskalnici in sicer smo uporabili različne izraze za opis temperaturne odvisnosti gostote elastomerov, toplotnih kapacitet in toplotnih prevodnosti, slednji pa so se uporabili v energijski bilanci. Ta je bila rešena s pomočjo kvazi-eksaktne metode in eksplicitne metode končnih razlik. Eksperimenti na pilotni stiskalnici so bili izvedeni za naravni kavčuk, butadienski kavčuk, hidrogenirani nitrilbutadienski kavčuk, izoprenski kavčuk in kloroprenski kavčuk. Medtem ko so bili eksperimenti na pilotni stiskalnici uporabljeni za modelno določitev temperaturno odvisnih toplotnih prevodnosti ter parametrov teh odvisnosti, se je za določitev temperaturno odvisne gostote elastomerov uporabila piknometrija in za določitev toplotne kapacitete diferenčna dinamična kalorimetrija. Izračunane in eksperimentalne temperature so se dobro ujemale skozi celotno preiskovano temperaturno območje med 20 in 200 °C. Razen tega so se določeni parametri temperaturne odvisnosti termodinamskih količin dobro ujemali s parametri drugih ne-elastomernih polimerov. Izdelani model skupaj z določenimi parametri se lahko uporabi za širok razpon elastomerov in obratovalnih pogojev pri njihovi predelavi ali

pa se celo združi z drugimi vidiki specifičnega procesa oziroma produkta, kot sta kinetika in mehanika (*POT3*).

Preučevanje elastomernih nanokompozitov: Preučevali smo nanokompozite, pripravljene iz hidrogeniranega nitrilbutadienskega kavčuka (HNBR) kot polimerne matrice in montmorilonita (MMT) oziroma različnih organsko modificiranih montmorilonitov (OMMT) kot polnil. Praktični del je obsegal pripravo HNBR-MMT (OMMT) nanokompozitov s tehniko mešanja v talini in dodajanjem dikumil peroksida (DCP) kot vulkanizacijskega sredstva. Mehanske, termične in druge fizikalno-kemijske lastnosti nanokompozitov smo preučevali z uporabo diferenčne dinamične kalorimetrije, rentgenske difraktometrije, dinamične mehanske analize ter določevanjem trdote po metodi Shore A. Ugotovili smo, da s podaljševanjem časa mešanja dosegamo boljše razslojevanje silikatnih plasti v polimerni matrici, a smo navsezadnje omejeni z elastomerom in polnilom, kajti po določenem času mešanja, se porazdelitev polnila v matrici ni več bistveno spreminjala. Splošna ugotovitev je bila, da s polnilom in v kakršnemkoli deležu slednjega dosežemo odlične mehanske in termične lastnosti HNBR-MMT (OMMT) nanokompozitov. Te lastnosti pa so najboljše, v kolikor modifikator MMT-ja po polarnosti dobro ustreza elastomerni matrici, saj pride ob povišani temperaturi do zamreževanja med verigami elastomera in modifikatorja (*POT9*).

Testiranje mehanskih lastnosti gume in gumenih kompozitov: Preučevali smo dinamične mehanske lastnosti vulkaniziranega elastomera (FKM) v širokem območju temperatur in strižnih pogojev. Za namen študije smo kot analizni metodi uporabili dinamično mehansko analizo in diferenčno dinamično kalorimetrijo. Razvili smo model, ki popisuje viskoelastično obnašanje FKM pri različnih temperaturah. Z uporabo razvitega algoritma smo z modelom popisali eksperimentalne točke. Tako smo dobili diskretni relaksacijski spekter za FKM pri dveh različnih temperaturah, Williams-Landel-Ferry (WLF) parametre in aktivacijske energije, potrebne za napoved faktorjev pomika oz. parametrov, ki nastopajo v WLF in Arrheniusovi zvezi. Model smo uporabili za popis eksperimentalno pridobljenih vrednosti strižnega elastičnega modula in faktorja izgub v odvisnosti od temperature. Ugotovili smo, da WLF enačba odlično popiše eksperimentalne točke v območju steklastega prehoda, medtem ko Arrheniusova zveza napoveduje prehiter padec elastičnega modula med steklastim prehodom. S pomočjo uporabe predhodno izračunanih parametrov, ki nastopajo v WLF in Arrheniusovi zvezi, smo izdelali še glavne krivulje za napoved viskoelastičnega obnašanja materiala v širokem frekvenčnem območju. Razviti model je uporaben za različne elastomere in omogoča napoved njihovega frekvenčno-temperaturnega obnašanja na osnovi dinamičnih mehanskih lastnosti pridobljenih z izotermnimi ali dinamičnimi eksperimenti z nizko hitrostjo segrevanja (*POT6, POT1*).

Sinteza, karakterizacija in optimizacija procesa sinteze formaldehidnih smol: Študirali smo kinetiko sinteze fenol-formaldehidnih smol v bazičnem mediju. Izvedli smo več sintez pri različni temperaturah, z različnimi razmerji med fenolom in formaldehidom in z različnimi razmerji med fenolom in natrijevim hidroksidom. Sestava smole je namreč odvisna od razmerja monomerov, vrste in količine katalizatorja in temperature med sintezo. Za spremljanje reakcij med sintezo in določanje koncentracij nezreagiranih monomerov smo uporabljali ReactIR analizni sistem, ki omogoča določanje IR spektrov v reakcijskem sistemu med sintezo. Koncentracijo hidroksilnih ionov smo določali preko meritev pH vrednosti raztopine. Koncentracija hidroksilnih ionov izražena kot funkcija reakcijskega časa, je bila popisana s polinomom šeste stopnje. Na osnovi predlaganega reakcijskega mehanizma je bil zapisan kinetični model. Za reševanje seta kinetičnih enačb, zapisanih v diferencialni obliki, smo uporabili Rosenbrockovo numerično metodo. Kinetični parametri so bili določeni na osnovi eksperimentalno določene spremembe koncentracije fenola in formaldehida med sintezo. Na takšen način je bilo mogoče izračunati tudi spremembe koncentracij petih hidroksimetifenolnih specij z reakcijskim časom.

Za posamezne reakcije so bile izračunane aktivacijske energije in predeksponentni faktorji. Pravilnost matematičnega modela je bila potrjena s primerjavo eksperimentalno določenih koncentracijskih profilov za fenol in formaldehid z izračunanimi za različna molska razmerja (*POT4*).

Raziskave sinteze melaminsko-formaldehidnih smol in tehnologije priprave melaminskih pen: V okviru raziskav s področja melaminsko formaldehidnih (MF) smol in melaminsko formaldehidnih (MF) pen smo proučevali sintezo in karakterizacijo MF smol, ter različne postopke priprave MF pen. V okviru študija sinteze MF smol smo proučevali vpliv začetnega molskega razmerja med melaminom in formaldehidom, ter vpliv pH na potek sinteze in končne lastnosti produkta. S pomočjo ReactIR analiznega sistema smo »in line« spremljali reakcije sinteze MF smole. S pomočjo NMR tehnike, smo izmerili kemijske premike ^{1}H in ^{13}C NMR signalov pomembnih funkcionalnih skupin ter posneli tudi FT-RAMAN spektre. S kombinacijo navedenih analitskih tehnik smo določili časovni potek naraščanja množine etrskih mostičkov in vsebnost posameznih funkcionalnih skupin v končnih produktih MF smol. Iz MF smole smo pripravili MF pene. Proučevali smo vpliv dodane količine aditivov in načina priprave MF pen na njihove končne lastnosti. Pene smo pripravljali v konvencionalni peči in mikrovalovni pečici. Parametri, ki smo jih spreminjali pri pripravi MF pen, so bili: delež katalizatorja, delež emulgatorja, temperatura konvencionalne peči, čas penjenja v mikrovalovni pečici in moč mikrovalovne pečice. MF penam smo določili gostoto, ter izmerili njihove mehanske lastnosti. Ugotovili smo, da ima gostota pen bistven vpliv na mehanske lastnosti MF pen. Na gostoto pen pomembno vpliva količina dodanega katalizatorja. Najnižje gostote so imele pene z nižjim deležem katalizatorja. Pene pripravljene v konvencionalni peči pri nižji temperaturi so imele višje gostote kot pene pripravljene pri višji temperaturi. Pene pripravljene v mikrovalovni pečici so bile bistveno bolj homogene in so imele nižje gostote kot pene pripravljene v konvencionalni peči (*POT11*).

Sinteza, karakterizacija in optimizacija procesa sinteze akrilatnih lepil: Pri raziskavah suspenzijske polimerizacije za sintezo mikrosfernih, na pritisk občutljivih (PSA) akrilatnih lepil smo ovrednotili vpliv molekulske mase in reakcij zamreževanja na njihove lepilne lastnosti. Osnovne lastnosti kot so kompozicija kopolimera, mikrostruktura, molekulska masa in porazdelitev molekulske mase spadajo med najbolj pomembne parametre, pri čemer se njihov vpliv na lastnosti PSA lepil odraža direktno, kot tudi indirektno preko vpliva na temperaturo steklastega prehoda (T_g) ter na reološke lastnosti polimera. Pri sintezah akrilatnih polimerov pogosto prihaja, zaradi intramolekularnega in intermolekularnega prenosa aktivnega mesta na verigo polimera, do nastanka razvejanih polimerov z dolgimi stranskimi verigami, kar vodi v nastanek gel faze. Poleg tega na količino gel faze vpliva tudi prepletenost linearnih polimernih molekul, ki je pogojena z molekulsko maso sintetiziranih polimernih verig ter stopnjo zamreženja. Molekulsko maso sintetiziranega polimera smo uravnavali z dodatkom reagenta za prenos verige (1-dodecil merkaptan), stopnjo zamreženja z uporabo di oziroma triakrilatnega monomera (butandiol diakrilat in trimetilolpropan triakrilat). Ugotovili smo, da so adhezivne lastnosti sintetiziranih lepil močno odvisne že od majhnih koncentracij dodanih reagentov. Poleg tega smo adhezivne lastnosti modificirali tudi s sintezo nanokompozitnih PSA materialov, pri čemer smo pri sintezi uporabili različne vrste in količine modificiranih montmorilonitnih (MMT) glin. S sintezo nanokompozitnih materialov smo zelo izboljšali odpornost na delovanje strižnih sil (*POT10*).

Sinteza, karakterizacija in optimizacija procesa sinteze enokomponentnih poliuretanskih lepil: Študirali smo sintezo in lastnosti enokomponentnih uretanskih lepil. NCO terminirane uretanske prepolimere smo sintetizirali iz difenilmetan-4,4'-diizocianata in različnih dvofunkcionalnih polipropilenglikolnih poliolov ter njihovih mešanic. Sintezo smo zasledovali s FTIR-ATR

spektroskopijo, ki omogoča merjenje IR spektrov reakcijske mešanice med sintezo. Ugotovili smo, da je bila hitrost nastanka uretanske skupine višja pri višji koncentraciji NCO skupin v reakcijski mešanici. Povprečna molekulska masa in viskoznost po Brookfieldu sta naraščali s padajočim NCO/OH razmerjem pri nespremenjeni sestavi poliola. Ko je bil za sintezo uporabljen poliol z višjo molekulsko maso je nastal prepolimer z višjo molekulsko maso in z nižjo viskoznostjo po Brookfieldu, kar smo pripisali večji vsebnosti mehkih poliolnih segmentov v prepolimerni verigi. Molekulska masa prepolimerov je vplivala na njihovo temperaturo steklastega prehoda, še posebej, ko je bil prepolimer pripravljen iz poliola z nižjo molekulsko maso. Z naraščanjem vsebnosti poliola z višjo molekulsko maso in padanjem vsebnosti poliola z nižjo molekulsko maso v poliolni fazi je temperatura steklastega prehoda prepolimera padala. Pri nizkih NCO/OH razmerjih je trdnost spoja lepila z lesom v testirancih les-lepilo-les naraščala z naraščajočo vsebnostjo prostih NCO skupin v prepolimeru. Nad določeno kritično vsebnostjo prosti NCO skupin pa se je trdnost spoja poslabšala na račun večje krhkosti lepila. Lepila z višjo vsebnostjo poliolov z višjimi molekulskimi masami in nižjo vsebnostjo prostih NCO skupin so imela daljši čas zamreženja, kar smo potrdili tudi z dinamično mehansko analizo (*POT2*).

Raziskave na področju ekspanzijskega injekcijskega stiskanja: Razvoj ekspanzijskega injekcijskega stiskanja kot nove tehnologije za proizvodnjo tankih polimernih delov zahteva poznavanje lastnosti in obnašanja polimernih talin v procesu hitrega visokotlačnega stiskanja in ekspanzije. Za namen tovrstnih raziskav smo razvili nov »in-line« merilni sistem za aparaturo za ekspanzijsko injekcijsko stiskanje, ki deluje pri visokih tlakih in temperaturah, ki se dosegajo v industrijski proizvodnji. Merilna šoba opremljena s hidravlično pomičnimi zaporami in kontaktnimi hitro odzivnimi tlačnimi in infrardeče temperaturnimi senzorji omogoča merjenje kompresije in ekspanzije polimernih talin v merilnem kanalu pri različnih začetnih pogojih. Rezultati meritev za proti udarcem odporen polistiren (HIPS) in poliamid so pokazali, da je temperatura polimerne taline linearno naraščala s kompresijskim tlakom in je odvisna od hitrosti stiskanja. Med ekspanzijo polimera je bil zabeležen primerljiv padec temperature, iz česar sledi, da ni pomembne izgube energije v reverzibilnem procesu. Rezultate meritev smo primerjali z modificirano dvoobmočno Taitovo enačbo stanja. Analiza prilagajanja krivulj na proizvajalčeve specifikacije materialov je potrdila, da so rezultati meritev v skladu z napovedmi modela, tudi pri že zelo visokih hitrostih stiskanja.

BIOKEMIJSKO INŽENIRSTVO IN BIOTEHNOLOGIJA

Kontinuirni proces biotransformacije steroidov: Z uporabo peletne oblike nitaste glive *Rhizopus nigricans,* ki jo lahko obravnavamo kot naravno imobilizirano biomaso, smo uspeli postaviti kontinuirni proces 11α-hidroksilacije progesterona v laboratorijskem mešalnem bioreaktorju. Za povečanje topnosti steroida smo uporabili β-ciklodekstrin in s tem povišali hitrost hidroksilacije steroida. Na osnovi razvitega matematičnega modela smo potrdili predhodno opredeljene kinetične parametre in uspeli napovedati obnašanje bioreaktorja. Z uporabo peletov različnih velikosti smo proučili vpliv morfologije na kinetiko reakcije in ugotovili, da je hitrost biotransformacije sorazmerna celokupni zunanji površini peletov, kar nakazuje prisotnost encimskega sistema za hidroksilacijo le v zunanjih plasteh aglomeratov glive *Rhizopus nigricans* (*KIŽ2*).

Ekstrakcija steroidov v mikroreaktorju: V mikrokanalu smo pri različnih pretokih študirali kontinuirno ekstrakcijo progesterona in 11α-hidroksiprogesterona, reaktanta in produkta biotransformacije, vključene v proizvodnjo kortikosteroidov. Teoretično izračunane parametre prenosa snovi smo potrdili z modelom in eksperimentom nestacionarne šaržne ekstrakcije progesterona brez mešanja. Razvili smo tudi tridimenzionalni model, ki je vključeval difuzijo in konvekcijo ob upoštevanju hitrostnega profila za laminarni tok dveh vzporednih kapljevin v mikrokanalu,

s katerim amo lahko analizirali eksperimentalne podatke in napovedali obnašanje mikroreaktorja pri stacionarnih pogojih. Za numerično rešitev kompleksnega sistema enačb smo uporabili neekvidistantne končne razlike. Dobili smo zelo dobro ujemanje eksperimentalnih podatkov z modelom brez kakršnegakoli prileganja parametrov. Na osnovi učinkovite ločitve obeh faz na izstopu iz mikrokanala in visoke učinkovitosti ekstrakcije smo ugotovili, da so ekstrakcijske enote submilimetrskih dimenzij obetavno sredstvo za razvoj integriranega sistema 11α-hidroksilacije progesterona z glivo *Rhizopus nigricans* v obliki peletov (*KIŽ16*).

Biokatalitske reakcije v mikroreaktorju: V okviru naših raziskav na področju implementacije mikroreaktorjev v biotehnologiji smo proučevali encimsko katalizirano oksidacijo 3, 4-dihidroksifenil-L-alanina tako v klasičnem šaržnem reaktorju, kjer smo opredelili kinetični model reakcije in njegove parametre, kot tudi v mikroreaktorju, kjer smo v bistveno krajših časih dosegli zelo visoke konverzije. Rezultate raziskav, ki smo jih izvedli v sodelovanju s Fakulteto za kemijsko inženirstvo in tehnologijo v Zagrebu, smo predstavili na več mednarodnih kongresih.

Študija encimsko katalizirane sinteze izoamil acetata: Izvedli smo tudi študijo encimsko katalizirane sinteze izoamil acetata, ki je eden najpomembnejših estrov, uporabljenih v prehrambeni industriji. Reakcijo, katalizirano z lipazo, smo najprej študirali v dvofaznem sistemu voda-heksan v klasičnem šaržnem reaktorju, nato pa smo esterifikacijo uspešno izvedli tudi v kontinuirnem procesu v mikroreaktorju, kjer je reakcija potekala neprimerno hitreje, hkrati pa je omogočala recikel encima v vodni fazi. V nadaljevanju smo obravnavano sintezo acetata izvedli tudi v enofaznem sistemu z uporabo ene od ionskih kapljevin. Na osnovi dobrih rezultatov sinteze v izbrani ionski kapljevini v mikroreaktorju nameravamo postaviti integriran »lab on a chip« sistem s kontinuirno ekstrakcijo v zaporedno vezanem mikrokanalu. Rezultate raziskav smo predstavili na več mednarodnih kongresih.

Submerzna biosinteza ekstra in intracelularnih učinkovin, kultivacija glivine biomase ekstra in intracelularnih učinkovin na trdnem gojišču, gojenje gliv na odpadkih lesno predelovalne industrije na eksperimentalni farmi gob, izolacija in purifikacija glivinih polisaharidov in testiranje aktivnosti indukcije citokinov na človeških celičnih linijah: Z optimizacijo postopka submerznega gojenja v bioreaktorju in postopka gojenja glivine biomase na trdnem gojišču smo uspeli ustvariti večje količine micelija. Paralelno s tem so tekle osnovne raziskave produkcije aktivne glivine biomase v smislu gojenja gob na eksperimentalni farmi, ki smo jo za raziskave ustanovili s sofinancerjem ZRS Bistra v Podkorenu. Iz vseh oblik pridobljene glivine biomase smo ekstrahirali glivine ekstra in intracelularne polisaharide. Polisaharidne frakcije smo frakcionirali in opravili čiščenje imunomodulatornih učinkovin, ki so v končnem obdobju projekta predvidene za testiranje na celičnih kulturah. Tu gre za komplekse β-glukanov (β -1,6 glukani in β -1,3 glukani) in proteinov, ki so topni v vodi in se obarjajo z etanolom, zato tudi postopki priprave imunomodulatornih polisaharidnih frakcij temeljijo na ekstrakciji v vodne medije in obarjanju z etanolom. Izolirane substance smo prečistili sedaj pa poteka testiranje imunomodulatornega učinkovanja (indukcija interlevkina, interferona, tumor nekrozirajočega faktorja) in vitro na človeških celičnih linijah (PBMC) (*KIŽ22*).

Postopki za zvišanje produkcije glicerola – Uporaba termošoka na vcepku kvasovk *Saharomyces cerevisia:* V alkoholni fermentaciji vinskega mošta smo izdelali in patentirali nov postopek temperaturnega šoka na vcepek vinskih kvasovk in njegov učinek na metabolizem *Saccharomyces cerevisiae.* Pri tem smo razvili nov originalni tehnološki postopek, ki omogoča produkcijo visokih dobitkov glicerola v vinih. Ugotovili smo, da je možno s toplotno obdelavo vcepka kvasovk povišati biosintezo glicerola za več kot 90 %. Ta postopek je možno uporabiti tudi v velikem industrijskem merilu, saj ne zahteva večjih aparativnih sprememb in omogoča enostavno izvedbo (*KIŽ3, KIŽ10*).

OKOLJSKO INŽENIRSTVO IN APLIKACIJE

Bioremediacija: Ugotovili smo, da dodana sladkor in dušik povečata encimske aktivnosti, od lesnih nosilcev pa se je najbolje izkazala bukev. Z različnimi gojišči lahko vplivamo na razmerja posameznih encimskih aktivnosti. Od izbranih barvil se je najhitreje razbarvalo barvilo RBBR, najobstojnejše pa je bilo barvilo RO16 (*KIŽ20*).

DRUGI RELEVANTNI DOSEŽKI

MODELIRANJE IN PROCESNO INŽENIRSTVO

Izolacijske plošče na osnovi ekspandiranega perlita: Uspešnost dosedanjih raziskav je privedla do prenosa laboratorijskih in pilotnih spoznanj na industrijski nivo in iskanja optimalnih tehnoloških rešitev pri industrijski proizvodnji novega izolacijskega materiala na osnovi ekspandiranega perlita, trenutno pa je v izdelavi poslovni načrt industrijske tehnologije za proizvodnjo novih izolacijskih produktov na osnovi ekspandiranega perlita.

Aplikativne raziskave na področju membranskih separacijskih tehnik: (*KIŽ38*).

POLIMERNO INŽENIRSTVO IN TEHNOLOGIJA

Razvoj testne aparature in metode za določanje abrazije zobatega pogonskega jermena: Na trgu so dostopni različni standardizirani instrumenti in metode, ki omogočajo merjenje abrazije različnih materialov. Posamezni obstoječi standardizirani instrumenti in metode so sicer primerni tudi za testiranje abrazijske odpornosti gumenih izdelkov, vendar niso primerni za hitro testiranje abrazijske odpornosti zobatega pogonskega jermena, saj ne omogočajo obremenjevanja jermena na način in pod pogoji, ki bi bili primerljivi z njegovo realno aplikacijo. Pri zobatem pogonskem jermenu je kritično mesto obrabe vdolbina med dvema zoboma. Na hitrost obrabe oz. mero abrazije ključno vplivajo številni dejavniki, kot so lokalne napetosti v materialu, segrevanje materiala in hitrost vrtenja jermenice. Namen raziskave je bil razviti testno napravo in ustrezne metode, ki bi omogočale merjenje abrazijske odpornosti zobatega pogonskega jermena. Naprava naj bi omogočala določevanje obrabe zobatega pogonskega jermena pri različnih obremenitvah z možnostjo spremljanja dviga temperature na mestu obremenitve. Razvita je bila laboratorijska testna aparatura in razvite so bile testne procedure, ki omogočajo merjenje abrazije zobatega pogonskega jermena na kritičnem mestu obrabe. Aparatura omogoča hiter test in hkrati dobro simulacijo pogojev pri aplikaciji jermena in je primerna predvsem za primerjalne teste med različnimi kvalitetami jermenov. Omogoča merjenje poškodbe na 0,01 mm natančno. Simuliranje različnih obremenitev je zagotovljeno z uporabo različnih uteži. Omogočeno je merjenje temperature na mestu obrabe (*POT13*).

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

Programme goals are presented according to five main research topic divisions: *Process engineering and modeling, Rheology and applications, Polymer engineering and technology, Bioengineering and biotechnology,* and *Environmental engineering.*

PROCESS ENGINEERING AND MODELING

In alkaline papermaking system sizing is often performed by the use of alkylketene dimer (AKD) type sizing agents. Although the key factor for developing sizing properties in paper is the reaction between AKD and cellulose during drying, good retention of size particles in the paper web is required as a prerequisite for later reaction. A mathematical model based on particle collision frequency has been used for the description of deposition kinetics of colloidal alkylketene dimer particles on pulp fibers.

The gas holdup database, obtained from a conventional bubble column, working with non-Newtonian liquids (aqueous xanthan and CMC solutions of different concentrations) with perforated plate as a gas distributor was analyzed with the *drift-flux model* and with the *slip velocity model*. The results were confronted with those predicted from the proposed correlations for liquid batch system and two-phase flow system.

The experimental study of the hydrodynamics of bubble column working with xanthan solutions (where sintered plate served as a gas distributor) was enriched with the measurements of gas holdup in the solutions of middle class concentrations. The qualitative tracer test was performed as well.

We continued with the research of nanofiltration in the system with organic solvents in order to concentrate active pharmaceutical compounds. Comparison between nanofiltration and evaporation has been made for the selected solvent and pharmaceutical compound.

RHEOLOGY AND APPLICATIONS

The influence of HL on mechanical properties of bitumen and bituminous mortar (mixture of filler and bitumen) was examined for two bitumen types: unmodified road bitumen B50/70 and polymer modified PmB II, which are most frequently used in Slovenia in the production of asphalt mixtures for wearing surfaces and wearing-close surfaces. The experimental work was carried out by using standard test-methods and rheological characterization. In bituminous mortars a part of filler was replaced with HL, the amount of HL varied from 0 to 20 wt.%. All the samples were examined before and after forced temperature ageing and after bituminous binder extraction (by trichloro-ethylene).

Rheological investigation of the landslide Slano Blato near Ajdovščina (Slovenia). In the last decade, first movements of the landslide were observed on Nov. 2000, reaching movements of 60–100 m/day. By means of geotechnical surveys on the landslide in 2004, rheological characterization of landslide material at different humidity was carried out. Even though this is not usual practice in geomechanical research work, it gave important information for further analysis of landslide stability. Numerical simulations of landslide stability were performed using the Burgher elasto-plastic model.

The object of the research on the mixing was to measure the velocity field in non-Newtonian fluids inside the mixing vessel with a six-bladed vane rotor. During mixing, the viscosity was determined by measuring the torque at different impeller speeds, and compared to rheologically obtained shear dependent viscosity.

An analysis of power consumption in mixing and dispersing of air into a shear thinning fluid in a standard cylindrical vessel stirred by a Rushton turbine was made by using aqueous solutions of CMC at $w = 0.5\%$ and $w = 1\%$ mass fraction and compressed air. The apparent viscosity which enabled the power vs. Reynolds number relation was calculated using the Metzner-Otto

method. A comparison of the power-consumption measurement resulted in single-phase mixing is in good agreement with the results found in literature.

POLYMER ENGINEERING AND TECHNOLOGY

Developments in these fields demand multi disciplinary basic and applied research, which includes polymer synthesis and characterization, polymer engineering, polymer material design and development of technology for material production. The programme goals were: to study the kinetics of vulcanization process and heat transfer during vulcanization process for different rubber blends and to describe them by mathematical modeling, to determine and to model the viscoelastic behavior of elastomeric systems in a wide range of temperatures and frequencies, to prepare, characterize and study the properties of nanocomposites, prepared from elastomers representing the polymer matrix and montmorillonite treated with modifier molecules as filler, to develop a testing apparatus for testing automotive timing belt abrasion resistance, to study and model the kinetics of phenol-formaldehyde and melamine-formaldehyde resins, to develop a technology for melamine foam production, to optimize the synthesis and product properties of acrylic microsphere pressure sensitive adhesives, to study the synthesis of one-component urethane adhesives and to design adhesive properties, and to develop a new in-line measurement system mounted to injection molding machine.

BIOENGINEERING AND BIOTECHNOLOGY

Based on our previous studies on the impact of bioprocess parameters on fungal morphology and estimation of kinetic parameters of progesterone biotransformation in the presence of β-cyclodextrin, we developed a continuous process of progesterone 11α-hydroxylation with *Rhizopus nigricans* pellets in a laboratory-scale stirred tank bioreactor. In order to develop an integrated system of progesterone biotransformation, a continuous ethyl acetate extraction of steroid biotransformation products was performed in a microchannel, which provides very efficient mass transfer and low consumption of chemicals.

Integration of the biocatalytic processes with microreactor technology has enormous potentials. Microstructured devices have demonstrated several advantages in (bio)chemical processes, especially due to a very large surface-area-to-volume ratio, connected with very effective heat and mass transfer, easier control of process parameters and new production concepts by numbering-up instead of scaling-up which results in the increase of production capacity. In recent years, a successful application of enzymatic microreactors has been reported, mainly in chemical analysis and kinetic studies. However, the potential of enzymatic microreactors to be used for industrial-scale synthesis and in environmental protection has not been exploited yet. Few enzymatic processes in microreactors have been reported, with only a few patents describing the construction of micro enzyme-reactors. The main goal of our recent studies is the implementation of microreactor technology in biocatalytic processes and definition of basic transport phenomena and fluid flow dynamics within microchannels using modern modeling. Furthermore, we intend to develop environmentaly-sustainable microreactor technologies, also by the use of ionic liquids, referred to as »Green solvents«. They have several favorable characteristics: negligible vapor pressure, excellent thermal stability, high capacity for dissolving a wide range of organic compounds, non-flammable properties, high conductivity, etc. However, their use in industrial processes is restricted due to high prices at the market, so the development of the processes with this solvent at microscale might be a promising alternative.

Research on pharmaceutically active compounds of *Grifola frondosa: Grifola frondosa* is lignin degradating organism, well established in research. Its highly active pharmaceutical compounds are one of the most active natural immunostimulants, interesting for modern pharmaceutical industry. Research of pharmaceutically active compounds of *Grifola frondosa* took place in three main directions : (1) Submerged cultivation on a liquid substrate in stirred tank reactor was optimized in relation of substrate composition as well as in process optimization, where a specific double-stage feed technology for high production of active fungal biomass was developed; (2) Solid state bioprocessing of secondary wastes from wood and agriculture industry wastes, as well as (3) Farming of mushrooms on agriculturual wastes on an experimental pilot mushroom farm. The goal of this research was to optimise various fermentation substrates for active biomass production. Protocols for effective isolation and purification of external and internal fungal polisaccharides were developed.

The research in pilot experiments on experimental farming using solid substrates based on wood and agriculture industry wastes: Extra- and intracellular polysaccharides were isolated from the active fungal biomass in all the three types of cultivation. Polysaccharide fractions were isolated and purified. Complexes of β-glucans (β -1,6 and β -1,3 glucans) were detected. Present research is going on in studying purified isolates, tested for their immunomodulatory activity by induction of interleukine, interferrone, TNF-α, tumor necrosis factor) in vitro in human peripherial mononuclear blood cells (PBMC).

Biochemical engineering in wine technology: Glycerol, as a secondary product of fermentation process, is one of the most relevant factors for premium wine quality. Its usual concentration in wines does not exceed 6 g l^{-1}. Because of its high specific gravity and viscosity, high concentrations of glycerol significantly contributes to fullness and complexity of dry wines. In research of new pathways for high glicerol production in wine technology a new method, based on heath shock of *Saccharomyces cerevisiae* suspension, was developed.

ENVIRONMENTAL ENGINEERING

There is a continuous research in the field of bioremediation. We studied enzyme activities MnP and Lac produced by *Ceriporiopsis subvermispora* in Kirk medium with additional sugar and nitrogen source, grown on various types of wooden support. The produced enzymes were used to study the decolourization of various synthetic dyes.

RESEARCH TOPICS

Process engineering and modeling:

- Applied process engineering research of first generation products based on phosphoric substances and product engineering research of the new generation 3E+C products
- Preparation of polymer-coated controlled release fertilizers
- Chelate synthesis for agrochemical purposes
- Biocide adsorption in powder formulations for agrochemical purposes
- Mathematical modeling of retention process in alkaline papermaking system
- Gas holdup in a conventional bubble column with perforated plate, working with non-Newtonian liquids
- Membrane separations – research of nanofiltration in systems with organic solvents

Rheology and applications:
- The influence of hydrated lime (HL) on mechanical properties of bitumen and bituminous mortar
- Rheological investigation of the landslide Slano Blato near Ajdovščina (Slovenia)
- Determining the velocity field in non-Newtonian fluids inside a mixing vessel with a six-bladed vane rotor
- An analysis of power consumption during mixing and dispersing of air into a shear thinning fluid in a standard cylindrical vessel stirred by a Rushton turbine

Polymer engineering and technology:
- Kinetic investigations during vulcanization process for different rubber blends and modeling
- Heat transfer investigations during vulcanization process for different rubber blends and modeling
- Synthesis, preparation and characterization of nanocomposite materials
- Testing of rubber and rubber composites
- Synthesis, characterization, modeling and optimization of the synthesis process of formaldehyde resins
- Research and development of a technology for the production of melamine foams
- Synthesis, characterization and optimization of the synthesis process of acrylic adhesives
- Synthesis, characterization and optimization of the synthesis process of one-component urethane adhesives
- Studies in the field of injection blow molding

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
- Submerged biosynthesis of extra and intracellular fungal polysaccharides
- Solid state fungal biomass cultivation and biosynthesis of intracellular fungal polysaccharides
- 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 peripherial mononuclear blood cells (PBMC)
- New technology for high glycerol production in wines
- Influence of heat shock of *Saccharomyces cerevisiae* inoculum on glycerol metabolism production in wine

Environmental engineering:
- Research in the field of bioremediation

SCIENTIFIC ACHIEVEMENTS

PROCESS ENGINEERING AND MODELING

Mathematical modeling of the retention process in alkaline papermaking system: In alkaline papermaking system sizing is often performed by the use of alkylketene dimer (AKD) type sizing agents. Although the key factor for developing sizing properties in paper is the reaction between AKD and cellulose during drying, good retention of size particles in the paper web is a prerequisite for later reaction. A mathematical model based on particle collision frequency is used for the description of deposition kinetics of colloidal alkylketene dimer particles on pulp fibers. A modified Langmuir equation was used to describe the retention process in terms of surface coverage, attachment and detachment rate constants. The values for equilibrium retention predicted by the model are in good agreement with experimental data. The analysis of surface charge in the system also suggests that the extent and efficiency of collisions between colloidal AKD size particles with fibers are one of the key factors for successful retention. Influence of shear on the retention process was also studied. The work was published in the article *KIŽ5*.

Gas holdup in a conventional bubble column with perforated plate, working with non-Newtonian liquids : The results of an extensive experimental study performed in a column with the perforated plate as the gas distributor indicted that in CMC solutions the gas holdup obeyed power-law dependency on the effective liquid viscosity, which yielded simple correlations for the prediction of gas holdup for both modes of operations. Both correlations over-estimate the gas holdup in xanthan solutions, though moderately in the liquid batch. It seems that xanthan solutions behave quite differently. Even though both types of solutions are viscoelastic and pseudoplastic in their nature, xanthan solutions exhibit weak jell behaviour, while CMC solutions exhibit polymer solution behaviour. The results were successfully published in an international journal (*KIŽ18*).

Membrane separations: The comparison between nanofiltration and evaporation showed that the concentration with nanofiltration is much cheaper.

RHEOLOGY AND APPLICATIONS

The influence of hydrated lime (HL) on the mechanical properties of bitumen and bituminous mortar: The most evident effect of HL in bituminous mortars was found to be on the shear viscosity. Presence of HL in the filler stiffens the mixture, the level of mixture hardening depend on the amount of HL and on bitumen type. Higher increase in viscosity was found for unmodified road bitumen B50/70. The variation in low temperature properties of bituminous mortars was less prominent up to a certain amount of HL, however, higher amounts of HL change the properties. HL in bituminous mortar inhibited the process of oxidation. This effect was more pronounced in polymer modified bitumen. Mechanical properties of both types of bitumen, extracted from the different bituminous-filler mixtures, did not change significantly. The results are published in *KIŽ32*.

Rheological investigation of the landslide Slano Blato near Ajdovščina (Slovenia): Using the visco-plastic Burghers model the rheological characteristics of gravel landslide mass were studied. Taking into account the rheological properties of the materials at different landslide locations, the model allowed for describing the actual situation on the landslide. In this way, when the smallest particle fractions had a water content between 35 and 40%, we were able to simulate even the largest deformations. The results were published in *KIŽ7*.

Velocity field in non-Newtonian fluids inside the mixing vessel with a six-bladed vane rotor: The velocity field was determined by LDA measurements at twelve points inside the mixing vessel. It was observed that axial and radial component of the velocity were insignificant at all measurement points. The results showed the periodic nature of tangential component of the velocity, which was also confirmed by computer-aided visualization method (*KIŽ19*).

An analysis of power consumption in mixing and dispersing of air into a shear thinning fluid in a standard cylindrical vessel stirred with a Rushton turbine: When air is dispersed into a shear thinning fluid, an obvious reduction of power consumption can be noticed especially at higher impeller speeds and gas flow rates, which is more noticeable in w = 0.5% than in a 1.0% CMC solution. In fact, the dissipated mixing power depends on gas-filled cavity structures behind the blades, which affected the impeller pumping efficiency. All experimental flow regimes were analyzed and depicted in a generalized flow regime map as Froude vs. Flow number dependence. Structure development was shown from high-effective to low-effective operation, e.g. complete dispersion and bubble column operation, respectively. Mixing power was found to be independent from the airflow rate at low Reynolds numbers. A comparison of the values measured in air-dispersion and the results from correlations found in literature confirm a general trend of impeller power reduction.The results were published in *KIŽ4*.

POLYMER ENGINEERING AND TECHNOLOGY

Kinetic investigations during vulcanization process for different rubber blends and modeling: The vulcanization kinetics of conventional blend types was studied where polybutadiene (BR) and polyisoprene (NR) rubber were chosen as an example. Kinetic parameters in vulcanization of NR and BR compound were obtained using regression analysis of the developed model and based on experimental data from differential dynamic calorimetry and dynamic mechanical analysis measurements. Due to the temperature dependence of kinetic parameters, the Arrhenius law dependence of the parameters was assumed. Pre-exponential coefficients and activation energies were thus calculated according to this relationship. Model results exhibited good correspondence with experimental data obtained from isothermal differential dynamic calorimetry and dynamic mechanical analysis measurements. Taking into consideration the variation of heat transfer during the scorch period, and temperature dependence of the rate constants of the key cross-linking reactions it was deduced that the largest scorch time is achieved at 50 weight % of polybutadiene loading in blends. Moreover, at this level of loading the high rate of cross-linking and a relatively low rate of reversion were observed as well (*POT3*).

Heat transfer investigations during vulcanization process for different rubber blends and modeling: The research objective was to study the heat transfer through elastomers. Heat transfer is often of a great importance in several elastomer processing unit operations and even more so in the case of any variety of vulcanization process although it is seldom treated equally important as cross-linking kinetics. Heat transfer in several elastomers was studied on a pilot-scale mold utilizing various expressions for describing temperature-dependent elastomer densities, heat capacities and thermal conductivities, which were applied in the governing heat equation. The latter was solved by means of quasi-exact and explicit finite difference algorithms. Molding experiments were performed for natural rubber, polybutadiene, hydrogenated butadiene-acrylonitrile copolymer, polychloroprene and polyisoprene. Whereas the molding experiments were applied to determine the temperature-dependent thermal conductivities, the temperature dependent densities and heat capacities were determined separately using pycnometry and differential dynamic calorimetry, respectively. The experimental and the predicted temperatures were in good agreement throughout the entire examined temperature range between 20 and

200 °C. Moreover, the determined parameters of the temperature-dependent thermodynamic quantities may be correlated to the parameters of other, non-elastomeric polymers. The developed model along with its determined parameters may be readily applied for a wide range of elastomers and processing operating conditions or even combined with other aspects of a certain operation, such as kinetics or mechanics (*POT3*).

Synthesis, preparation and characterization of elastomeric nanocomposite materials: The research objective was to study the properties of nanocomposites, prepared from hydrogenated nitrile-butadiene copolymer (HNBR) representing the polymer matrix and montmorillonite (MMT) or montmorillonite, treated with modifier molecules (OMMT) as a filler. The experimental part consisted of HNBR-MMT (OMMT) nanocomposite preparation utilizing melt compounding technique and dicumyl peroxide (DCP) addition, the latter being a cross-linking agent. Mechanical, thermal and other chemo-physical properties of the nanocomposites were studied using differential dynamic calorimetry, X-ray diffraction, dynamic mechanical analysis and hardness determination, utilizing Shore A method. We found out that upon prolongation of the blending time, a higher degree of exfoliation of silicate layers is achieved within the polymer matrix; nevertheless, one is limited by the elastomer and the filler, as after certain blending time lapse the distribution of filler within the matrix cease to vary noticeably. A general observation was that by adding the filler, regardless of its loading, excellent mechanical and thermal properties of the HNBR-MMT (OMMT) were obtained. The characteristics were the best when MMT modifying molecules corresponded well with the elastomer matrix polarity, because the cross-linking among elastomer and modifier chains occurs upon elevating the temperature (*POT9*).

Testing dynamic mechanical properties of rubber and rubber composites: The dynamic mechanical properties of a vulcanized fluoroelastomer (FKM) were studied over a range of temperatures and shear frequencies. Dynamic mechanical analysis and differential scanning calorimetry were used for the purpose of the study. A model was developed in order to describe FKM's viscoelastic behavior at various temperatures. The model was fitted to experimental data using an algorithm, which was developed for this purpose. As a result, the FKM discrete relaxation spectrum at two reference temperatures was obtained, as well as the Williams-Landel-Ferry (WLF) equation parameters or the activation energy equivalent, depending on the type of equation used for the prediction of the shift factors. Further on, the model was applied on storage modulus and loss tangent values obtained from the experiments, during which the temperature increased linearly. It was observed that the WLF equation fits well the results during the glass transition, while the Arrhenius-type relationship predicted too rapid decrease of the storage modulus during the glass transition. Master curves were constructed using the previously calculated WLF parameters and the activation energy equivalent. The developed model may be readily applied for the prediction of the numerous FKM compounds' frequency-temperature behavior using the dynamic mechanical properties obtained from either isothermal or low linear heating rate program measurements (*POT6, POT1*).

Synthesis, characterization, modeling and synthesis process optimization of formaldehyde resins: Phenol-formaldehyde resins are products which are synthesized by step polymerization of phenol and formaldehyde under alkaline or acidic conditions. Two prepolymer types are obtained depending on the pH: novolacs in an acidic pH region, and resols in alkaline region. Three reaction sequences must be considered: formaldehyde addition to phenol, chain growth or prepolymer formation and finally the cross linking or curing reaction. Within the aim of our research work, the kinetics of phenol-formaldehyde prepolymers catalyzed by sodium hydroxide at various temperatures was studied. Several reactions were conducted with different phenol to formaldehyde, as well as phenol to sodium hydroxide ratios. The phenolic resin com-

position depends on the monomer ratio, type and amount of the catalyst, reaction conditions (temperature), and residual free monomers. The ReactIR system was used to monitor the reaction as well as to determine residual free phenol and formaldehyde. Changes in the concentrations of phenol and formaldehyde with the reaction time were determined. The concentration value of the hydroxide ion, [OH^-] can be obtained by measuring the pH value of reaction mixture. The concentration of the hydroxide ion, [OH^-], expressed as a function of reaction time, was fitted by the six-order polynomial to the experimental data. On the basis of the proposed reaction mechanism the kinetic model was written down. To solve the set of proposed kinetic equations (in a differential form) the Rosenbrock numeric method was employed. The kinetic parameters were obtained by adjusting the experimental evolution of phenol and formaldehyde during the synthesis. Using this method the changes in the concentrations of five species of hydroxymethylphenols with the reaction time can also be calculated. The activation energy and preexponential factor have been calculated for individual reactions. The accuracy of the mathematical model was confirmed by comparing experimental concentration profiles of formaldehyde and phenol with the calculated ones (using the estimated kinetic parameters) for different molar ratios. The experimental tendencies are in agreement with the results of the model (*POT4*).

Research and development of the production technology of melamine foams: The synthesis and characterization of melamine- formaldehyde (MF) resin and different procedures of preparing melamine formaldehyde foams have been investigated. In the context of synthesis, we have varied the initial molar ratio between melamine and formaldehyde and the initial pH values. Syntheses have been »in line« monitored by ReactIR analytic system. MF resins have also been analyzed by FT – RAMAN technique and NMR technique by measuring intensities of ^{1}H and ^{13}C NMR signals of important functional groups. With the combination of these analytical techniques, the rising quantity of ether bridges during the synthesis and quantity of important functional groups in the final MF resin were determined. MF foams were prepared from MF resins. The influence of the amount of additives and the procedure for MF foam preparation on final foam properties has been investigated. Foams were prepared in a conventional oven and in a microwave oven. The parameters which were varied were: percent of catalyst, percent of emulsifier, temperature of conventional oven, time of foaming in microwave oven and the power of microwave oven. The density and the mechanical properties of foams were determined. It was found out that there is a correlation between the density and the mechanical properties of foams. The amount of catalyst vitally influences the foam density and its mechanical properties. The foams with the lowest densities were the ones, which were prepared using lower catalyst amounts. Foams prepared in conventional oven at lower temperature, exhibited relatively higher densities in comparison to those, prepared at higher temperatures. Better homogeneity was achieved utilizing microwave oven even though the foams had generally lower densities (*POT11*).

Synthesis, characterization and synthesis process optimization of acrylic adhesives: The influence of polymer molecular weight and crosslinking reactions on the adhesion properties of microsphere pressure sensitive adhesives (PSA) was investigated. Inherent polymer properties, such as copolymer composition, polymer microstructure and molecular weight have major direct impacts on the adhesion properties of the microsphere PSA, and indirectly influence their physical properties (e.g., T_g) and thus also the rheological properties of polymer. An important problem regarding the use of the acrylic monomer system is the formation of a gel phase during the polymerization process. Recent studies show that the acrylate chain-growth kinetics can be complicated by the intermolecular and intramolecular (backbiting) transfer to polymer and this process leads to the formation of gel phase in the adhesive. In addition to the in-

tramolecular transfer to polymer, the amount of both crosslinked polymer molecules, as well as highly entangled and coiled polymer molecules contribute to the formation of the gel phase in the adhesive. Molecular weight of the adhesive was modified with the employment of chain transfer agent (n-dodecylmercaptane) and the crosslinking reactions were induced by the addition of either di or triacrylate acrylic monomers (butanediol diacrylate and trimethylolpropane triacrylate). The results of our study showed, that all adhesive properties strongly depend even on low concentrations of added modifiers. In addition to this synthesis procedure, we also modified the adhesion properties of PSA's by the synthesis of polymer nanocomposite materials with different amounts of various montmorilonitte (MMT) clays. By this procedure, we significantly improved shear properties of the microsphere PSA's (*POT10*).

Synthesis, characterization and optimization of the synthesis process of one-component urethane adhesives: The synthesis and structure-property relationships of one-component urethane adhesives were studied. NCO-terminated urethane prepolymers were prepared from monomeric diphenylmethane-4,4'-diisocyanate, difunctional polypropyleneglycol polyols and their mixtures. The syntheses were monitored by in-line FTIR-ATR spectroscopy. The rate of the urethane group formation increased with increasing free isocyanate (NCO) concentration in the bulk. The average molecular weight and Brookfield viscosity of the urethane prepolymers increased with decreasing the NCO/OH ratio in fixed polyol composition. When prepolymers contained longer polyol segments, the average molecular weight increased, while Brookfield viscosity decreased due to higher content of soft segments, which made urethane chains more flexible. The average molecular weights of prepolymers affected their glass transition temperature values, particularly when prepolymers had shorter soft segments. By increasing the content of polyol with higher molecular weight and decreasing the content of polyol with lower molecular weight, the glass-transition temperature decreased. At lower NCO/OH ratios the rigidity and stiffness of the adhesive bond in wood-to-wood specimens increased with increasing free NCO content, whereas beyond a critical free NCO content, high stiffness caused the decrease of adhesion strength. The cure time of adhesives increased by increasing polyol molecular weight and decreasing free NCO content (*POT2*).

Research in the field of injection blow molding: The development of expansion injection molding as new technology for producing thin plastic parts has raised questions about polymer melt behavior in the process of rapid high-pressure compression and expansion. To be able to investigate those phenomena, a new in-line measurement system mounted to injection molding machine has been developed which can work under high pressures and temperatures encountered during industrial production. A measuring nozzle, equipped with hydraulically driven closing bolts, and contact, fast-response pressure and infrared temperature sensors enabled us to measure the compression and expansion of polymer melts in the measuring channel at different starting conditions. The results presented for high impact polystyrene and polyamide show that the polymer melt temperature rise is linearly dependent on the compression pressure as well as it is dependent on compression speed. A comparable effect of temperature fall has been recorded during the polymer expansion, which means that there is no noticeable loss of dissipation energy during this reversible process. Measurements have been compared with modified 2-domain Tait equation of state. Curve fitting analysis to manufacturer's material data show that measurements fit well with the model, even at very high compression speeds.

BIOENGINEERING AND BIOTECHNOLOGY

Continuous biotransformation of progesterone: A pelleted morphological form of *Rhizopus nigricans*, which might be regarded as a naturally immobilized biomass, enabled the develop-

ment of a continuous process of progesterone 11α-hydroxylation in a laboratory scale stirred tank bioreactor. β-cyclodextrin was used to enhance steroid solubility in aqueous transformation media and consequently to increase the rate of steroid hydroxylation. Batch and continuous processes were performed by pellets of different average diameters, ranging from less than 1 mm to 7.5 mm. Mathematical model simulations of both operation modes confirmed the previously defined biotransformation kinetics, based on Michaelis-Menten equation. A decrease in overall hydroxylation rate was noticed when pellets larger than 5 mm were used, which correlated with the lower area of the outer surface of agglomerates, where enzyme inducement presumably took place. The work was published in the article *KIŽ2*.

Steroid extraction in a microchannel system: In this project we studied the continuous ethyl acetate extraction of progesterone and 11α-hydroxyprogesterone, the reactant and the product of the biotransformation step involved in corticosteroid production in a microchannel at different flow velocities. In addition, non-steady state batch extraction without mixing was performed and modelled in order to verify the theoretically predicted parameters. In order to analyze experimental data and to forecast microreactor performance, a three-dimensional mathematical model with convection and diffusion terms was developed by considering the velocity profile for laminar flow of two parallel phases in a microchannel at steady-state conditions. For the numerical solution of a complex equation system, non-equidistant finite differences were used. Very good agreement between model calculations and experimental data was achieved without any fitting procedure. Due to the efficient phase separation and high extraction yields obtained, the micro scale extraction units were found to be a promising tool for the development of an integrated system of 11α-hydroxylation of progesterone by *Rhizopus nigricans* in the form of pellets. The work was published in the article (*KIŽ16*).

Biocatalytic reactions in a microchannel system: Enzymatic oxidation of 3, 4-dihydroxyphenyl-L-alanine (L-DOPA) with laccase from *Trametes versicolor* was investigated. The highest enzyme activity at pH 5.4 and at 25 ºC was found. The reaction kinetics and the effect of dissolved oxygen concentration on the reaction rate were evaluated. A mathematical model, comprised of double-substrate Michealis-Menten kinetics and mass balances for L-DOPA and dissolved oxygen concentrations, was developed in order to describe and predict the process of L-DOPA oxidation. Kinetic parameters, V_{m}, $K_{\mathrm{m}}^{\mathrm{L\text{-}DOPA}}$ and $K_m^{O_2}$ were estimated and experimentally verified by a set of experiments with constant additional aeration for different initial concentrations of L-DOPA and dissolved oxygen. A significant increase in the reaction rate was established at a higher oxygen concentration in the inlet gas. The influence of dissolved oxygen concentration on L-DOPA conversion was investigated using the developed model. The work was presented on scientific conferences and the original scientific article ”Modelling of L-DOPA oxidation catalyzed by laccase” by M. Tišma, P. Žnidaršič-Plazl, I. Plazl, B. Zelić and Đ. Vasić-Rački is in press in *Chem. Biochem. Eng. Q.* Further studies of the investigated reaction were done in a microreactor, where high conversions of L-DOPA (up to 87%) were achieved at very short residence times (τ = 110 s). A two-dimensional mathematical model, composed of convection, diffusion, and enzyme reaction terms, was developed in order to describe and predict microreactor behaviour. The work was presented at several scientific conferences.

Enzyme catalyzed synthesis of isoamyl acetate in a microreactor: An enzyme catalyzed synthesis of isoamyl acetate, which is one of the most employed flavors in food industries, was studied in a microreactor. Lipaze-catalysed reaction in a two-phase water-n-hexane system was first studied in a classical batch reactor, while further studies were performed in a continuous process in a microreactor, where the reaction was much faster and enabled the reuse of the enzyme. The investigated esterification was performed also in a one-phase system with

a selected ionic liquid. Based on previous good results of isoamyl acetate synthesis of this solvent, we intend to develop an integrated »lab on a chip« system with continuous product extraction in a consecutive microchannel. The results were presented at several international conferences.

Submerse biosynthesis of extra and intracellular fungal polysaccharides, solid state fungal biomass cultivation and intracellular fungal polysaccharides biosynthesis, farming cultivation of *Grifola frondosa* fungal fruit bodies on wood and agriculture industry secondary wastes, isolation and purification of extra- and intracellular fungal polysaccharides and in-vitro testing of immunostimulatory activities of isolates by induction of cytokines in human peripherial mononuclear blood cells (PBMC): *G. frondosa* mycelium biomass with pharmaceutically active polysaccharides was produced by: (1) solid-state cultivation in polyethylene bags, (2) solid-state cultivation in a horizontal stirred tank bioreactor. Slovenian isolate of *G. frondosa* was used in all experiments. The experiments showed the importance of the substrate moisture content. The above experimental results confirmed that *G. frondosa* biomass can be successfully produced by both cultivation methods: by solid-state cultivation in polyethylene bags and by solid-state cultivation in a horizontal stirred tank bioreactor. Both cultivation methods were suitable for the production of fungal polysaccharides, including β-D-glucans, which are the most important active compounds of *G. frondosa*. Compared to submerged cultivation, solid state cultivation seems to have some advantages: higher biomass yield, lesser susceptibility to bacterial infections, and a potential of using agricultural wastes as effective lignocellulosic substrates for the production of *G. frondosa* biomass. This research is presented in *KIŽ30*. *G. frondosa* biomass and its pharmaceutically active polysaccharides were produced by submerged cultivation in a liquid medium a 10-L bioreactor. Slovenian isolate of *G. frondosa* was used in all experiments. *G. frondosa* mycelium was cultivated in a liquid medium – in Erlenmayer flasks and in a 10-L mixing bioreactor. The above experimental results confirmed that *G. frondosa* biomass can be successfully produced by submerged cultivation on synthetic media. Submerged cultivation proved to be suitable for the production of fungal polysaccharides, including β-D-glucans, which are the most important active compounds of *G. frondosa*. This research is presented in *KIŽ31*.

New technology for high glycerol production in wines – Influence of heat shock of *Saccharomyces cerevisiae* inoculum on glycerol metabolism production in wine: A heat shock was applied to *Saccharomyces cerevisiae*. This is a new and easy method for high glycerol production in large scale wine production. The cells subjected to heat shock acquire resistance to various stresses. Fast changes in fermentation temperature result in a rapid response in yeast metabolism. Yeast cells pushed out of their balance and forced into new temperature environment, started a pronounced glycerol secretion to reach another stable redox balance suitable for further microbial growth. A fast temperature change induced activation of the enzyme triose phosphate isomerase which displayed higher affinity to dihydroxyacetone phosphate than to glycerol aldehyde 3-phosphate, which was converted in a two-step reaction to glycerol. The work was published in the article *KIŽ3*.

ENVIRONMENTAL ENGINEERING

Bioremediation: It was found that the addition of sugar and nitrogen can increase enzyme activities- while beech-wood proved to be the best support material. Different media compostiton causes various ratios between enzyme activities. The highest decolourization rate was achieved with RBBR, while the most resistant dye was RO16 (*KIŽ20*).

OTHER RELEVANT ACHIEVEMENTS

PROCESS ENGINEERING AND MODELING

New insulation material based on expanded perlite: The results of the research so far on a new insulation material, based on expanded perlite on the laboratory and pilot level were successfully implemented on the industrial level. Simultaneously, relevant process parameters were optimized. At present the company is developing a business plan for industrial technology production of new insulation materials based on expanded perlite.

Applied research in the field of membrane separations: (*KIŽ38*).

POLYMER ENGINEERING AND TECHNOLOGY

Development of a testing apparatus and method for testing abrasion resistance of the automotive timing belt: Nowadays, there are several standardized instruments and methods for abrasion testing of different materials and products available on the market. Some of them are suitable for rubber and rubber composite testing, however they are not suitable for testing specific applications such as automotive timing belt. They do not enable a testing procedure which would simulate the loading mode and conditions during real application, where the critical point for product failure represents the space between two teeth. There are several factors affecting the abrasion, such as local stresses in the material, material heating and belt pulley speed. The scope of the research was to develop a testing apparatus, which would allow to determine the timing of belt abrasion resistance under different loadings conditions and to measure the temperature on the abrasion point. With the developed testing apparatus and methods a satisfactory simulation of real use conditions can be achieved. The test provides for fast and accurate measurements of the groove depth and temperature at the damaged site (*POT13*).

ENOTE SKUPNE DEJAVNOSTI

Center za NMR spektroskopijo visoke ločljivosti, Enota za tehnično podporo, Enota za športno vzgojo, Knjižnica fakultete, Založba fakultete in Tajništvo (dekanat) fakultete, so enote, ki izvajajo skupno dejavnost fakultete.

CENTER ZA NMR SPEKTROSKOPIJO

je del nacionalnega centra za NMR spektroskopijo, ki vključuje tudi enoti na Kemijskem inštitutu in Inštitutu Jožef Štefan. Kot infrastrukturni center je nemenjen za znanstveno-raziskovalno, razvojno in izobraževalno dejavnost. Dejavnosti se izvajata na podlagi nacionalnega raziskovalnega in razvojnega programa ter nacionalnega programa visokega šolstva (diplomske, magistrske naloge in doktorske disertacije).

ENOTA ZA TEHNIČNO PODPORO

skrbi za vzdrževanje pedagoške in raziskovalne opreme, za izdelavo in popravilo laboratorijske steklovine.

ENOTA ZA ŠPORTNO VZGOJO

skrbi za izvajanje športne vzgoje študentov fakultete.

KNJIŽNICA FAKULTETE

skrbi za izposojo, nabavo in katalogizacijo strokovne literature ter za vnos biografskih in bibliografskih podatkov visokošolskih učiteljev, znanstvenih delavcev in sodelavcev fakultete v COBISS.

ZALOŽBA FAKULTETE

skrbi za izdajo učbenikov in drugega strokovnega gradiva potrebega 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 2007
CHAIRS IN 2007

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
doc. dr. Nataša Gros

Asistenti / Assistants
dr. Robert Susič
dr. Tatjana Zupančič
doc. dr. Matevž Pompe
doc. dr. Helena Prosen
dr. Drago Kočar
dr. Irena Kralj Cigić
dr. Polonca Kralj
mag. Ivanka Keber

Raziskovalci / Researchers
izr. prof. dr. Matija Strlič (v dopolnilnem razmerju)
dr. Jana Kolar (v dopolnilnem razmerju)
Danijela Pucko, dipl. ing. kem. tehn.
Linda Csefalvayová, univ. dipl. kem.
dr. Martin Šala

Tehniki / Technicians

Zdenka Držaj

Jolanda Furlan

Mojca Žitko

Mladi raziskovalci Young Researchers	Mentor Mentor	Čas usposabljanja Programme Duration	Oblika usposabljanja Degree
Tanja Trafela	M. Strlič	2006–2011	doktorski študij / *PhD*
Gregor Arh	M. Veber	2006–2010	doktorski študij / *PhD*
Andrej Ščavničar	M. Pompe	2007–2012	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

Analitika in spektroskopija */Chemical Analyis and Spectroscopy* – VSŠ

Analizna kemija */ Analytical Chemistry* – VSŠ

Analizna kemija */ Analytical Chemistry* – UNI – Kemija / *Chemistry*

Analizna kemija */ Analytical Chemistry* – UNI – Kemijsko inženirstvo / *Chemical Engineering*

Avtomatizirana analiza */ Automated Analysis* – UNI

Instrumentalna analiza */ Instrumental Analysis* – UNI

Instrumentalne metode analize / *Instrumental Methods in Chemical Analysis* – UNI

Izbrana poglavja iz analizne kemije */ Selected Topics in Analytical Chemistry* – UNI

Kemija okolja */ Environmental Chemistry* – UNI

Kemijska analiza živil */ Chemical Analysis of Food* – UNI

Kemometrija v analizni kemiji */ Chemometrics in Analytical Chemistry* – UNI

Podiplomski programi / *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 Spectrometry*

Radiokemijske metode analize / *Radiochemical Methods of Analysis*

Separacijske metode v kemijski analizi / *Separations in Chemical Analysis*

Uvod v metode umetne inteligence v kemiji / *Fundamentals of Artificial Intelligence Methods in Chemistry*

IZVEN FKKT / EXTRAMURAL COURSES

Dodiplomski programi / *Undergraduate Programmes:*

Analizna kemija / *Analytical Chemistry* FFA – UNI in VSŠ

Analizna kemija / *Analytical Chemistry* PEF – UNI

Kemija okolja / *Environmental Chemistry* PEF – UNI

Podiplomski programi (UPŠ Varstvo okolja) / *Postgraduate Programmes (Environmental Protection)*

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

Kemijski procesi v okolju / *Chemical Processes in the 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; raziskave interakcij laserske svetlobe in organskih materialov; karakterizacija in stabilizacija organskih materialov, zlasti polimernih; študij elektrodnih procesov in razvoj tehnik adsorpcijske voltametrije; študij separacijskih in predkoncentracijskih postopkov (dializa, ekstrakcija na trdni fazi); analitika živil, zlasti vina, mesa in sira; analitika aminokislin; analitika sledov kovin; razvoj učinkovitih sistemov za vnos vzorcev v plamen in plazmo; atmosferska kemija ter konzervacijska kemija.

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 are chromatography, spectroscopy, electro analytical techniques, flow injection analysis, chemometry, automated analysis and robotics in analytical chemistry.

Research is oriented to studying interactions between metals and antibiotics, pesticides, humic substances, speciation studies, and the role of transition elements in oxidative media, studies of interactions of laser light with organic materials, characterization and stabilization of organic matter with special focus on polymers, studies of processes on electrodes and development of new techniques in adsorptive voltametry, studies of separation and preconcentration

procedures (dialysis, solid phase extractions), food analysis (wine, meat products and cheese), analysis of amino acids, development of sample introduction systems for atomic spectroscopy, atmospheric chemistry and chemical studies for the preservation of cultural heritage.

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

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 LC20 / *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 / *Shared with the National and University Library*:

– FT-NIR-MidIR-IR Perkin Elmer GX/ z DRIFT NIR celico / *with a DRIFT NIR Cell*
– Pretočni analizni sistem za viskozimetrijo / *Flow Analysis System for Viscometry*

Skupaj s KI / *Shared with the National Institute of Chemistry*:

– ICP-MS HP (Agilent) 4500
– ICP-MS-LA Agilent 7500 CE - UP-213

Skupaj z UNG in Kmetijskim inštitutom Slovenije / *Shared with the University of Nova Gorica and the Agricultural Institute of Slovenia*

– Sklopljeni tekočinski kromatograf/ masni spektrometer / *HPLC-MS /MS (Perkin Elmer Series 200, Applied Biosystems 3200 Q Trap)*

SODELOVANJE V CENTRIH ODLIČNOSTI / CENTERS OF EXCELLENCE

Center odličnosti: Nanoznanosti in nanotehnologija / *Center of Excellence: Nanosciences and Nanotechnology*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

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

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 – Information Source or Health Risk?*
Nosilec / *Principal Researcher*: M. Strlič
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*
Nosilec / *Principal Researcher*: M. Strlič
Sofinancer / *Co-sponsored by*: Zavod za varstvo pri delu

L1-6709 Transport atmosferskih onesnaževal preko Slovenije/ *Transport of Atmospheric Pollutants Across Slovenia (2003–2006)*

	Nosilec / *Principal Researcher*: M. Veber Sofinancer / *Co-sponsored by*: Agencija RS za okolje
V4-0996	Uporaba disperzijskih modelov pri načrtovanju izboljšanja in ohranjanja kakovosti zunanjega zraka / *Use of Dispersion Modelling for the Improvement of Ambient Air Quality* Nosilec / *Principal Researcher*: M. Pompe Sofinancer / *Co-sponsored by*: Ministrstvo za okolje in prostor RS
V4-0321	Fenolni potencial lokalnih kultivarjev sliv in češenj / *Phenolic Potential of Local Plum and Cherry Cultivars* Nosilec / *Principal Researcher*: M. Strlič Sofinancer / *Co-sponsored by*: Ministrstvo za kmetijstvo, gozdarstvo in prehrano RS

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

Socrates SF- EVTEK Institute of Art and Design
Koordinator / *Coordinator*: M. Strlič

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

SurveNIR SSPI-006594	Bližnje-infrardeča spektroskopija za pregled velikih zbirk / *Near Infrared Tool for Collection Surveying* Nosilec / *Principal Researcher*: M. Strlič
PaperTreat SSPI-006584	Presoja procesov masovnega razkislinjenja / *Evaluation of Mass Deacidification Processes* Nosilec / *Principal Researcher*: M. Strlič
InkCor EVK4-2001-00049	Stabilizacija papirja z železo-galnim črnilom / *Stabilisation of Iron Gall Ink Containing Paper* Nosilec / *Principal Researcher*: M. Strlič
MIP EVK4-2002-02001	Prehodne kovine v papirju/ *Transition Metals in Paper* Nosilec / *Principal Researcher*: M. Strlič
COST G7	*Artwork Conservation Using a Laser* Nosilec / *Principal Researcher*: M. Strlič

SI/03/B/F/PP-176012	*Hands-On Approach to Analytical Chemistry for Vocational Schools* Nosilec / *Principal Researcher*: N. Gros
COST E41	*Analytical Tools with Applications in Wood and Pulping Chemistry* Nosilec / *Principal Researcher*: M. Strlič
COST D42	*Chemical Interactions between Cultural Artefacts and Indoor Environment – EnviArt* Nosilec / *Principal Researcher*: M. Strlič
Eureka 3843	*Advanced Laser Renovation of Old Paintings, Paper, Parchment and Metal Objects* Nosilec / *Principal Researcher*: M. Strlič
FOOD – CT – 2006 -016264 EU 6. OP	*Traditional European Food (TRUEFOOD)* Nosilec / *Principal Researcher*: M. Pompe

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Hrvaška *Slovenia – Croatia*	Študij interakcije pesticidov z anorganskimi in organskimi snovmi v tleh / *Studies of Interactions between Pesticides and Inorganic and Organic Constituents in Soil* Nosilec / *Principal Researcher*: L. Zupančič-Kralj
Slovenija – Hrvaška *Slovenia – Croatia*	Nastanek, transport in razgradnja fotooksidantov na področju Mediterana / *Formation, Transport and Degradation of Photooxidants in the Mediterranean Region* Nosilec / *Principal Researcher*: M. Pompe
Slovenija – Italija *Slovenia – Italy*	Razvoj mikro nedestruktivnih spektroskopskih analiznih tehnik za študij razpada organskih materialov / *Development of Non- and Microdestructive Spectroscopic Analytical Techniques in Studying Degradation of Organic Materials.* Nosilec / *Principal Researcher*: M. Strlič
Slovenija – ZDA *Slovenia – USA*	Kvantitativna ocena tveganja pri tradicionalnih izdelkih živil / *Quantitative Risk Assessment of Traditional Food Products* Nosilec / *Principal Researcher*: M. Pompe

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UREDNIK / EDITOR

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KATEDRA ZA ANORGANSKO KEMIJO
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prof. dr. Peter Bukovec
izr. prof. dr. Boris Čeh
prof. dr. Alojz Demšar
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Aleš Knez
Urška Levec
Igor Ponikvar
Vinko Volk

Mladi raziskovalci Young Researchers	Mentor Mentor	Čas usposabljanja Programme Duration	Oblika usposabljanja Degree
Simona Medvešček	A. Meden	2003–2010	doktorski študij / *PhD*
Katarina Demšar	A. Meden	2006–2011	doktorski študij / *PhD*
Matej Smrkolj	A. Meden	2006–2008	doktorski študij / *PhD*
Jerneja Šauta Ogorevc	P. Bukovec	2006–2011	doktorski študij / *PhD*
Marta Kasunič	A. Golobič	2007–2012	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

Splošna kemija I / *General Chemistry I* – VSŠ
Splošna kemija / *General Chemistry* – UNI
Kemija in kemijska tehnologija / *Chemistry and Chemical Technology* – VSŠ
Anorganska kemija / *Inorganic Chemistry* – UNI in VSŠ
Anorganska kemija II / *Inorganic Chemistry II* – UNI
Bioanorganska kemija / *Bioinorganic Chemistry* – UNI
Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UNI
Izbrana poglavja iz anorganske kemije / *Selected Topics in Inorganic Chemistry* – UNI
Kemija kompleksov / *Chemistry of Complexes* – UNI
Kristalna kemija / *Crystal Chemistry* – UNI
Metodika anorganskih eksperimentov / *Methodology of Inorganic Experiments* – UNI

Podiplomski programi / *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

Dodiplomski programi / *Undergraduate Programmes*

Kemija / *Chemistry* FS – UNI
Kemija / *Chemistry* NTF – UNI in VSŠ
Kemija / *Chemistry* FMF – UNI in VSŠ
Osnove kemije / *Fundamentals of Chemistry* FGG – UNI
Kemija z osnovami biokemije / *Chemistry with Fundamentals of Biochemistry* BF – UNI
Anorganska kemija / *Inorganic Chemistry* FFA – UNI
Anorganska kemija / *Inorganic Chemistry* NTF – UNI
Anorganska kemija / *Inorganic Chemistry* BF – UNI
Anorganska kemija / *Inorganic Chemistry* PEF – UNI
Bioanorganska kemija / *Bioinorganic Chemistry* BF – UNI
Strukturna kemija / *Structural Chemistry* PEF – UNI
Kemija lesa / *Wood Chemistry* BF – UNI

Podiplomski programi / *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 Applicatios 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*
- Študij nanosa in strukture tankih plasti / *Studies of Thin Film Deposition*
- Razvoj ionskih hranilnikov / *Development of Ionic Containers*
- Termična analiza / *Thermal Analysis*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

- I. Turel, sourednik / *Co – Editor,* 2006 -, *Metal-Based Drugs*, Hindawi Publishing Corporation
- I. Turel, regionalni urednik / *Regional Editor* of *"Molecules", A Journal of Synthetic Organic Chemistry and Natural Product Chemistry*
- A. Demšar, sourednik / *Co-Editor*, *Acta Chimica Slovenica*

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

- I. Leban, sopredsednik organizacijskega odbora 17. slovensko-hrvaškega srečanja kristalografov / *Chair of the Organising Committee of the 17th Slovenian-Croatian Crystallographic Meeting*

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«, eksperimentlano predavanje za popularizacijo kemije / *"Researcher's Night" – Demonstration Lecture for the Popularization of Chemistry*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

– Modularni sistem za termično analizo – Mettler Toledo (TGA/SDTA 851, DSC 822, HP DSC 827) / *Modular System for Thermal Analysis – Mettler Toledo*
– Modularni sistem za termično analizo – Perkin Elmer (TGA7, DTA7) / *Modular System for Thermal Analysis – Perkin Elmer*
– HPLC kromatograf / *HPLC Chromatograph*
– Guinierjeva kamera ENRAF-NONIUS FR 552 / *Guinier Camera ENRAF-NONIUS FR 552*
– Polarizacijski mikroskop / *Polarisation Microscope*
– Stereomikroskop / *Stereomicroscope*
– Difraktometer za monokristale Nonius Kappa CCD / *Single-Crystal Diffractometer Nonius Kappa CCD*
– Difraktometer za monokristale Nonius CAD 4 / *Single-Crystal Diffractometer Nonius CAD 4*
– Visoko ločljivi rentgenski praškovni difraktometer s $CuK_{\alpha 1}$ radiacijo (50 % solastništvo s Kemijskim inštitutom / *High Resolution X-ray Powder Diffractometer*
– Spektrometer Perkin Elmer 2000 FT-IR / *Perkin Elmer 2000 FT-IR Spectrometer*
– Spektrometer Perkin Elmer 1720 X / *Perkin Elmer 1720X Spectrometer*
– Spektrometer UV/VIS/NIR Lambda 19 / *UV/VIS/NIR Lambda 19 Spectrometer*
– Termoanalizator Mettler 2000C / *Thermoanalyser Mettler 2000C*
– Suha komora MBraun Unilab / *Dry Box MBraun Unilab*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

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

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L1-6334	Nanokompozitni tanki filmi in pigmenti za industrijo premazov / *Nanocomposite Thin Films and Pigments for Coatings* Nosilec / *Principal Researcher*: P. Bukovec Sofinancer / *Co-sponsored by*: Helios Domžale d.d.
L2-7521	Uporaba novih materialov iz recikliranih odpadnih surovin in gradbenih odpadkov v gradbeništvu / *Reuse of Materials from Recycled Construction Waste Materials* Nosilec / *Principal Researcher*: P. Bukovec Sofinancer / *Co-sponsored by*: Cinkarna Celje d.d., Štore Steel d.o.o.
M2-0106	Samočistilni fotokatalitski premazi in prevleke / *Self-Cleaning Photocatalytical Coatings* Nosilec: / *Principal Researcher:* P. Bukovec Sofinancer / *Co-sponsored by*: Ministrstvo za obrambo RS
M5-0147	Razvoj učnih sredstev za ugotavljanje varstva pred požarom / *Development of Learning Means Used for Fire Protection* Nosilec / *Principal Researcher*: P. Bukovec Sofinancer / *Co-sponsored by*: Ministrstvo za obrambo RS

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI V RS / COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS IN SLOVENIA

- Melamin d.d.: Termična analiza kompozitov (letna pogodba) / *Thermal Analysis of Composites (Annual Contract*)

  Nosilec / *Principal Researcher:* N. Bukovec
- Krka d.d.: Letna pogodba (ekspertne storitve) / *Annual Contract (Expert Services)*
- Salonit d.d.: Letna pogodba (kvantitativne fazne analize) / *Annual Contract (Quantitative Phase Analyses)*

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 the Faculties and Schools: Life-Long Learning of Science Teachers*
Koordinator projekta: Fakulteta za kemijo in kemijsko tehnologijo / *Coordination of the Project: Faculty of Chemistry and Chemical Technology*
Vodja projekta / *Head of the Project*: N. Bukovec
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* Nosilec / *Principal Researcher*: S. Grabner
COST 540	*Photocatalytic Technologies and Novel Nanosurfaces Materials* Članica upravnega odbora /*Steering Committe Member*: R. Cerc Korošec
LIMNOTOP (LIFE-ENVIRONMENT)	*The Sustainable Rehabilitation of the Landfill Site* Nosilec / *Principal Researcher*: P. Bukovec
EURODEMO EU 6. OP	*European Platform for Demonstration of Efficient Soil and Groundwater Remediation* Nosilec / *Principal Researcher*: M. Zupančič
COST D39	*Ruthenium Anticancer Compounds* Nosilec /*Principal Researcher*: I. Turel

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Avstrija *Slovenia – Austria*	Koordinacijski polimeri: od načrtovanja zgradbe do uporabnih materialov / *Coordination Polymers: From Crystallization to the Possible Application* Nosilec / *Principal Researcher*: I. Leban
Slovenija – Hrvaška *Slovenia – Croatia*	Encimska kataliza – modelni sistemi: prenos protona v vodikovih vezeh z nizko energijsko bariero / *Enzyme Catalysis – Model Systems: Proton Transfer in Low Barrier Hydrogen Bonds* Nosilec / *Principal Researcher*: A. Meden
Slovenija – Češka *Slovenia – Czech Republic*	Novi mešani organokovinski aluminijevi-titanovi(IV) fosfati, fosfonati, fosfinati in fluoridi / *New Mixed Organometallic Aliminium-Titanium(IV) Phosphates, Phosphonates, Phosphinates and Fluorides* Nosilec / *Principal Researcher*: A. Demšar

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

– Prof. Jiři Pinkas, Masaryk University Brno, Češka, *Ultrasound in the Synthesis of Nanoparticles*, November 2007

BIBLIOGRAFIJA 2007 / REFERENCES 2007

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

AK1. ZUPANČIČ JUSTIN, Maja, ZUPANČIČ, Marija. Boron in irrigation water and its interactions with soil and plants: an example of municipal landfill leachate reuse = Bor v namakalni vodi in njegove interakcije s tlem in rastlinami: primer ponovne uporabe izcedne vode odlagališča komunalnih odpadkov. *Acta agric. Slov.*. [Tiskana izd.], 2007, letn. 89, št. 1, str. 289-300, graf. prikazi. [COBISS.SI-ID 28883973]

AK2. LAH, Nina, LEBAN, Ivan, GIESTER, Gerald. A new copper(II) basic sulfate : poly-[3-aminopyridinium [mu][sub]3-hydroxido-di-[mu][sub]3-sulfato-bis[aquacopper(II)]]. *Acta crystallogr., C Cryst. struct. commun.*, 2007, vol. C63, no. 5, str. m222-m224, ilustr. [COBISS.SI-ID 28608261]

AK3. PEVEC, Andrej, KOZLEVČAR, Bojan, GAMEZ, Patrick, REEDIJK, Jan. Hexakis-[mu]-chlorido-dichloridobis[(3, 5-dimethyl-pyrazol-1-yl)acetic acid-[kappa][sup]2N,N']tetracopper(II) : an unexpected neutral bis-pyrazolyl ligand in tetracopper(II) complex. *Acta crystallographica. E, Structure Reports*, 2007, vol. E63, no. 2, str. m514-m516, Graf. prikazi. [COBISS.SI-ID 28303109]

AK4. LEBAN, Ivan, RUDAN TASIČ, Darja, LAH, Nina, KLOFUTAR, Cveto. Structures of artificial sweeteners : cyclamic acid and sodium cyclamate with other cyclamates. *Acta crystallogr., B Struct. sci.*, 2007, vol. B63, no. 3, str. 418-425, ilustr. [COBISS.SI-ID 28619269]

AK5. BIČEK, Ajda, TUREL, Iztok, KANDUŠER, Maša, MIKLAVČIČ, Damijan. Combined therapy of the antimetastatic compound NAMI-A and electroporation on B16F1 tumour cells in vitro. *Bioelectrochemistry*. [Print ed.], 2007, vol. 71, no. 2, str. 113-117, ilustr. [COBISS.SI-ID 6153812]

AK6. KOKALJ, Anton, DOMINKO, Robert, MALI, Gregor, MEDEN, Anton, GABERŠČEK, Miran, JAMNIK, Janko. Beyond one-electron reaction in Li cathode materials : designing Li[sub]2Mn[sub]xFe[sub](1-x)SiO[sub]4. *Chem. mater.*. [Print ed.], 2007, vol. 19, no. 15, str. 3633-3640. [COBISS.SI-ID 3734554]

AK7. OVERGAARD, Jacob, TUREL, Iztok, HIBBS, David E. Experimental electron density study of a complex between copper(II) ant the antibacterial quinolone family member ciprofloxacin. *Dalton trans. (2003. Print)*, 2007, no. 21, str. 2171-2178. [COBISS.SI-ID 28628997]

AK8. BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. Synthesis and transformation of methyl 2-(6-hydroxy-2-phenyl-pyrimidin-4-yl)acetate : simple preparation of pyrimidines with heterocyclic substituents. *Helv. Chim. Acta*, 2007, vol. 90, no. 9, str. 1737-1744, graf. prikazi. [COBISS.SI-ID 28919813]

AK9. MODEC, Barbara, DOLENC, Darko, BRENČIČ, Jurij. New molybdenum(V) complexes based on the {Mo[sub]2O[sub]4}[sup](2+) structural core with esters or anions of malonic and succinic acid. *Inorg. Chim. Acta*. [Print ed.], 2007, vol. 360, no. 2, str. 663-678, graf. prikazi. [COBISS.SI-ID 28869637]

AK10. MALAVAŠIČ, Črt, BRULC, Blaž, ČEBAŠEK, Petra, DAHMANN, Georg, HEINE, Niklas, BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Combinatorial solution-phase synthesis of (2S,4S)-4-acylamino-5-oxopyrrolidine-2-carboxamides. *J. comb. chem.*, 2007, vol. 9, no. 2, str. 219-229. [COBISS.SI-ID 28465925]

AK11. PEZDIRC, Lidija, BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Combinatorial solution-phase synthesis of alkyl (1S*,2S*,3R*,5R*,6R*)-1-alkyl-3-aryl-6-benzoylamino-1-hydroxy-7- oxo-5-phenylhexahydropyrazolo[1,2-a]pyrazole-2-carboxylates. *J. comb. chem.*, 2007, vol. 9, no. 4, str. 717-723. [COBISS.SI-ID 28752389]

AK12. LEOVAC, Vukadin M., JOKSOVIĆ, Milan D., DIVJAKOVIĆ, Vladimir, JOVANOVIĆ, Ljiljana S., ŠARANOVIĆ, Žana, PEVEC, Andrej. Synthesis, spectroscopic and x-ray characterisation of a copper(II) complex with the Schiff base derived from pyridoxal and aminoguanidine : NMR spectral studies of the ligand. *J. inorg. biochem.*. [Print ed.], 2007, vol. 101, no. 7, str. 1094-1097, ilustr. [COBISS.SI-ID 28699397]

AK13. JAGLIČIĆ, Zvonko, ŠEGEDIN, Primož, ZLATIČ, Jernej, ZORKO, Andrej, PIRNAT, Janez, TRONTELJ, Zvonko. Magnetic interactions in a new copper(II) carboxylate complex. *J. magn. magn. mater.*. [Print ed.], 2007, vol. 310, iss. 2, str. 1444-1446. [COBISS.SI-ID 14258265]

AK14. DEMŠAR, Katarina, STARE, Jernej, MAVRI, Janez. Structure and vibrational dynamics of hydrogen bond in hydrogenbissulfate anion in the gas phase and in the solid state : a computational study. *J. mol. struct.*. [Print ed.], 2007, vol. 844/845, no. 1/3, str. 215-221. [COBISS.SI-ID 3743002]

AK15. VRBANIĆ, Daniel, MEDEN, Anton, NOVOSEL, Barbara, PEJOVNIK, Stane, UMEK, Polona, PONIKVAR, Maja, MIHAILOVIĆ, Dragan. Synthesis and characterization of Mo[sub]6S[sub](4.5)I[sub](4.5) nanowires. *J. nanosci. nanotechnol. (Print)*, 2007, vol. 7, no. 3, str. 982-985, Graf. prikazi. [COBISS.SI-ID 28263685]

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AK17. STEPHAN, Michel, ŠTERK, Damjan, MODEC, Barbara, MOHAR, Barbara. Study of the reaction of bulky aryllithium reagents with 3, 4-dimethyl-2,5-diphenyl-1,3,2-oxazaphospholidine-2-borane derived from ephedrine. *J. org. chem.*, 2007, vol. 72, no. 21, str. 8010-8018. [COBISS.SI-ID 3807258]

AK18. MOŠKON, Jože, DOMINKO, Robert, CERC KOROŠEC, Romana, GABERŠČEK, Miran, JAMNIK, Janko. Morphology and electrical properties of conductive carbon coatings for cathode materials. *J. power sources*. [Print ed.], 2007, vol. 174, no. 2, str. 683-688. [COBISS.SI-ID 3765530]

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AK21. KEVORKIJAN, Varužan, ŠKAPIN, Srečo D., JELEN, Marina, KRNEL, Kristoffer, MEDEN, Anton. Cost-effective synthesis of AlMgB[sub]14-xTiB[sub]2. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, iss. 2/3, str. 493-497. http://dx.doi.org/10.1016/j.jeurceramsoc.2006.04.114. [COBISS.SI-ID 10893078]

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AK23. CERC KOROŠEC, Romana, KAJIČ, Petra, BUKOVEC, Peter. Determination of water, ammonium nitrate and sodium nitrate content in "water-in-oil" emulsions using TG and DSC. *J. therm. anal. calorim.*, 2007, vol. 89, no. 2, str. 619-624, graf. prikazi. [COBISS.SI-ID 28865541]

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KATEDRA ZA BIOKEMIJO
CHAIR OF BIOCHEMISTRY

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prof. dr. Brigita Lenarčič

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
prof. dr. Brigita Lenarčič
izr. prof. dr. Metka Renko
prof. dr. Tamara Lah (v dopolnilnem razmerju)
izr. prof. dr.Vladka Čurin Šerbec (v dopolnilnem razmerju)

Asistenti / Assistants
doc. dr. Marko Dolinar
dr. Petra Prijatelj
dr. Nika Lovšin
dr. Vera Župunski
dr. Miha Pavšič

Tehnik / Technician
Matjaž Malavašič

Mlada raziskovalka Young Researcher	Mentor Mentor	Čas usposabljanja Programme Duration	Oblika usposabljanja Degree
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

Dodiplomski programi / *Undergraduate Programmes*

- Biokemija / *Biochemistry* – UNI
- Encimatika / *Enzymology* – UNI
- Tehnologija rekombinantne DNA / *Recombinant DNA Technology* – UNI
- Molekularna imunologija / *Molecular Immunology* – UNI
- Encimska tehnologija / *Enzyme Technology* – UNI
- Biološke membrane / *Biological Membranes* – UNI
- Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UNI
- Regulacija metabolizma / *Regulation of Metabolism* – UNI
- Biokemija raka / *Biochemistry of Cancer* – UNI
- Encimi / *Enzymes* – UNI

Podiplomski programi / *Postgraduate Programmes*

- Biološke makromolekule / *Biological Macromolecules*

IZVEN FKKT / EXTRAMURAL COURSES

Dodiplomski programi / *Undergraduate Programmes*

- Biokemija / *Biochemistry* FFA – UNI – Farmacija
- Biokemija / *Biochemistry* FFA – VSŠ – Laboratorijska biomedicina

Podiplomski programi (UPŠ Biomedicina) / *Postgraduate Programmes (Biomedicine)*

- Biokemija / *Biochemistry*
- Molekularna biologija / *Molecular Biology*

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

Raziskovalno delo članov katedre poteka v okviru Odseka za biokemijo in molekularno biologijo Instituta »Jožef Stefan« in to na treh raziskovalnih programih: Toksini in biomembrane, Proteoliza in njena regulacija ter Strukturna biologija.

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 membrane.

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. Z računalniškim modeliranjem smo določili potencialno imunogena mesta na površini mišjega imunoglobulina, nato pa na ravni DNA ta mesta mutiramo.

Kot novo področje smo začeli s pripravo DNA-konstruktov za analizo povezovalnih zaporedij v fuzijskih proteinih. Več pomnoženih humanih, bakterijskih in bakteriofagnih zaporedij z zapisi za biološko aktivne proteine bomo povezali z različnimi linkerji ter jih izrazili v bakterijah.

Research work of Chair members is organized within three research programmes based at the Jožef Stefan Institute: Toxins and Biomembranes, Proteolysis and its Regulation, and Structural Biology.

Research on toxinology focuses on 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 membrane.

Coworkers of 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 cell.

In cooperation with the National Blood Transfusion Center (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. By computer modelling, we determined potentially immunogenic sites on the surface of the murine immunoglobulin and mutated them on the DNA level.

As a new field of research we started preparing DNA constructs for the analysis of linker sequences in fusion proteins. Several human, bacterial and bacteriophage sequences coding for biologically active proteins will be joined by various linkers and expressed in bacteria.

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

V letu 2007 je doc. dr. Marko Dolinar sodeloval kot mentor študentske raziskovalne ekipe s področja sintezne biologije (v sodelovanju s Kemijskim inštitutom).

Skupina sedmih študentov Univerze v Ljubljani, med katerimi je bilo pet študentov Biokemije, je v času od maja do novembra izvedla raziskavo, s katero so dokazali, da bi bilo mogoče razvoj in širjenje okužbe z virusom HIV preprečiti na nov način. Temeljna ideja je bila, da je treba delovanje virusa zavreti z vplivom na virusno funkcijo, s čimer postane sistem neobčutljiv na mutacije. Ekipa je sodelovala na mednarodnem tekmovanju iGEM2007 v konkurenci 54 univerzitetnih ekip z vsega sveta in se na srečanju novembra 2007 na inštitutu MIT (Cambridge, ZDA) uvrstila med 6 najboljših, hkrati pa dosegla prvi mesto v kategoriji Medicina in zdravje in zlato medaljo za opravljene vse naloge.

Skupaj s prof. dr. Romanom Jeralo je doc. dr. Marko Dolinar prejel priznanje »Prometej znanosti za odličnost v komuniciranju«, ki ga podeljuje Slovenska znanstvena fundacija. V utemeljitvi so zapisali, da sta nagrado dobila za »požrtvovalno in uspešno komuniciranje s študenti o sintezni biologiji, oblikovanje ekipe ter za dosežene rezultate na svetovnem tekmovanju iGEM (International Genetically Engineered Machine Competition) v letih 2006–2007«.

In 2007 Asst. Prof. Dr. Marko Dolinar acted as a mentor of a student research team in the field of synthetic biology (in cooperation with the National Institute of Chemistry).

A group of seven undergraduate students, among them five Biochemistry students from our Faculty, carried out a 6-month research in which they proved that HIV infection and its spreading could be inhibited in a new way. The basic idea was that the virus should be inhibited by its function, by which the system unsusceptible to mutations. Our team competed among 54 teams from around the world at the international competition iGEM2007, held at MIT (Cambridge, MA) and turned out to be one of the best teams. We were one of six finalists, who won a golden medal for completing all the tasks and ranked first in the Health and Medicine track.

Together with Prof. Dr. Roman Jerala, Asst. Prof. Dr. Marko Dolinar was a recipient of the "Prometheus of Science for Excellency in Communication" awarded by the Slovenian Science Foundation. In their justification they wrote that the award was given for "unselfish and successful communication with the students in the field of synthetic biology, for building a team and for the results achieved at the world competition iGEM (International Genetically Engineered Machine Competition) in the years 2006 and 2007".

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*
- Aparatura za PCR / *PCR Apparatus*
- Naprave za elektroforezno analizo proteinov in Western prenos / *Instruments for Electrophoretic Separations of Proteins and Western Blot*

- 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 °C / *Freezer –80 °C*
- 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* Vodja programa / *Principal Researcher*: I. Križaj (IJS)
P1-0140	Proteoliza in njena regulacija / *Proteolysis and its Regulation* Vodja programa / *Principal Researcher*: V. Turk (IJS)
P1-0048	Strukturna biologija / *Structural Biology* Vodja programa / *Principal Researcher*: D. Turk (IJS)

BIBLIOGRAFIJA 2007 / REFERENCES 2007

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

BIO1. CUKJATI, Marko, KOREN, Simon, ČURIN-ŠERBEC, Vladka, VIDAN-JERAS, Blanka, RUPREHT, Ruth. A novel homozygous frameshift deletion c.471del of HFE associated with hemochromatosis. *Clin. genet.*, 2007, letn. 71, št. 4, str. 350-353. [COBISS.SI-ID 22999257]

BIO2. ČERNILEC, Maja, VRANAC, Tanja, HAFNER BRATKOVIČ, Iva, KOREN, Simon, COLJA VENTURINI, Anja, POPOVIĆ, Mara, JUNTES, Polona, ČURIN-ŠERBEC, Vladka. Identification of an epitope on the recombinant bovine PrP that is able to elicit a prominent immune response in wild-type mice. *Immunol. lett.*. [Print ed.], 2007, letn. 113, št. 1, str. 29-39. [COBISS.SI-ID 23195609]

BIO3. AGUIAR, Renato S., LOVŠIN, Nika, TANURI, Amilcar, PETERLIN, Boris Matija. VPR.A3A chimera inhibits HIV replication. *J Biol Chem*, 2008, issue 5, vol. 283, str. 2518-25. http://dx.doi.org/10.1074/jbc.M703097200. [COBISS.SI-ID 21302823]

BIO4. NOVINEC, Marko, GRASS, Robert N., STARK, Wendelin J., TURK, Vito, BAICI, Antonio, LENARČIČ, Brigita. Interaction between human cathepsins K, L, and S, Mechanism of elastinolysis and ihibition by macromolecular inhibitors. *J Biol Chem*, 2007, vol. 282, no. 11, str. 7893-78902. [COBISS.SI-ID 20683559]

BIO5. PLAZAR, Janja, ŽEGURA, Bojana, LAH TURNŠEK, Tamara, FILIPIČ, Metka. Protective effects of xanthohumol against the genotoxicity of benzo(a)pyrene (BaP), 2-amino-3-methylimidazo[4,5-f]quinoline (IQ) and tert-butyl hydroperoxide (t-BOOH) in HepG2 human hepatoma cells. *Mutat. res., Genet. toxicol. environ. mutagen.*, 2007, vol. 632, str. 1-8. [COBISS.SI-ID 1739855]

BIO6. OKEOMA, Chioma M., LOVŠIN, Nika, PETERLIN, Matija B., MARKI, Susan Ross. APOBEC3 inhibits mouse mammary tumour virus replication in vivo. *Nature (Lond.)*, 2007, vol. 445, no. 7130, str. 927-930. [COBISS.SI-ID 20903975

BIO7. KAC, Javor, PLAZAR, Janja, MLINARIČ, Aleš, ŽEGURA, Bojana, LAH TURNŠEK, Tamara, FILIPIČ, Metka. Antimutagenicity of hops (Humulus lupulus L.): bioassay-directed fractionationand isolation of xanthohumol. *Phytomedicine (Stuttg.)*, Available online 25 October 2007, 5 str., [in press]. http://dx.doi.org/10.1016/j.phymed.2007.09.008. [COBISS.SI-ID 1820495]

BIO8. STROJNIK, Tadej, RØSLAND, Gro Vatne, SAKARIASSEN, Per Oystein, KAVALAR, Rajko, LAH TURNŠEK, Tamara. Neural stem cell markers, nestin and musashi proteins, in the progression of human glioma: correlation of nestin with prognosis of patient survival. *Surg. neurol.*. [Print ed.], aug. 2007, vol. 68, no. 2, str. 133-143. [COBISS.SI-ID 2723903]

BIO9. ŽEGURA, Bojana, ZAJC, Irena, LAH TURNŠEK, Tamara, FILIPIČ, Metka. Patterns of microcystin-LR induced alteration of the expression of genes involved in response to DNA damage and apoptosis. *Toxicon (Oxford)*. [Print ed.], Available online 22 November 2007, 9 str., [in press]. http://dx.doi.org/10.1016/j.toxicon.2007.11.009. [COBISS.SI-ID 1820239]

KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

BIO10. CIGLIČ, Monika, FEKONJA, Ota, KOVAČ, Jernej, OBLAK, Alja, POHAR, Jelka, SKOČAJ, Matej, TKAVC, Rok, BENČINA, Mojca, PANTER, Gabriela, MANČEK KEBER, Mateja, DOLINAR, Marko, JERALA, Roman. Engineered human cells: say no to sepsis. *IET synth. biol. (Print)*. [Print ed.], 2007, vol. 1, no. 1/2, str. 13-16. [COBISS.SI-ID 3769882]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

BIO11. HAYRYAN, Shura, GHULGHAZARYAN, Ruben, POKLAR ULRIH, Nataša, ČURIN-ŠERBEC, Vladka, HU, Chin-Kun. Simulation of small peptide using combined Wang-Landau-transition matrix Monte Carlo algorithm. V: HANSMANN, Ulrich H. E. (ur.). *From computational biophysics to systems biology (CBSB07) : NIC Workshop 2007 : symposium, 02.-04. May 2007, Jülich : celebrating 20 years of NIC*, (NIC Series, vol. 36). Jülich: John von Neumann Institute for Computing (NIC), cop. 2007, str. 141-143. [COBISS.SI-ID 3330936]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

BIO12. STROJNIK, Tadej, KAVALAR, Rajko, LAH TURNŠEK, Tamara, STAUBAR, Rozalija, ZAJC, Irena. Proučevanje mehanizmov invazivnosti človeškega glioma na modelu v podganah : zaključno poročilo o rezultatih raziskovalnega projekta. Maribor: Splošna bolnišnica, 2007. 10, 6 f., ilustr. [COBISS.SI-ID 2620223]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

BIO13. LOVŠIN, Nika. *APOBEC3 cytidine deaminase suppresses replication MMTV retrovirus : invited talk*. Cambridge: MRC Laboratory of Molecular Biology, 7 Dec. 2007. [COBISS.SI-ID 21420839]

UREDNIK / EDITOR

BIO14. DOLINAR, Marko (ur.), STOKA, Veronika (ur.), TURK, Boris (ur.). *From single molecules to degradomics : book of abstracts*. Ljubljana: Jožef Stefan Institute, 2007. 149 str. ISBN 978-961-6303-92-7. [COBISS.SI-ID 233597440]

BIO15. *Pathology oncology research*. Lah, Tamara (član uredniškega odbora 1997-). Budapest: Tud. Kiadó. ISSN 1219-4956. [COBISS.SI-ID 21115]

BIO16. *Poročilo o delu - Nacionalni inštitut za biologijo*. Lah, Tamara (član uredniškega odbora 1995-). Ljubljana: Inštitut za biologijo, 199?-. ISSN 1408-3299. [COBISS.SI-ID 68115968]

BIO17. *Radiology and oncology*. Lah Turnšek, Tamara (član uredniškega odbora 2007-). Ljubljana: Slovenian Medical Society - Section of Radiology; [Zagreb]: Croatian Medical Association - Croatian Society of Radiology, 1992-. ISSN 1318-2099. [COBISS.SI-ID 32649472]

BIO18. *Raziskovalec*. Lah, Tamara (član uredniškega odbora 1993-). Ljubljana: Ministrstvo za znanost in tehnologijo Republike Slovenije, 1971-2000. ISSN 0351-0727. [COBISS.SI-ID 15966978]

KATEDRA ZA FIZIKALNO KEMIJO
CHAIR OF PHYSICAL CHEMISTRY

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Jože Koller

SODELAVCI KATEDRE / PERSONNEL

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prof. dr. Andrej Jamnik
prof. dr. Ksenija Kogej
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prof. dr. Ciril Pohar
prof. dr. Jože Škerjanc
prof. dr. Gorazd Vesnaver
prof. dr. Vojeslav Vlachy

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Matjaž Bončina
doc. dr. Janez Cerar
dr. Andrej Godec
doc. dr. Barbara Hribar Lee
Miha Lukšič
dr. Črtomir Podlipnik
dr. Iztok Prislan
doc. dr. Jurij Reščič
Bojan Šarac
dr. Matija Tomšič
dr. Tomaž Urbič

Raziskovalci / Resarchers
dr. Jožica Dolenc
mag. Irena Lipar

Strokovni sodelavec / Research Assistant
Aleksander Vrhovšek

Tehniki / Technicians
Anton Kelbl
Anton Kokalj
Cirila Peklaj

Mladi raziskovalci Young Researchers	Mentor Mentor	Čas usposabljanja Programme Duration	Oblika usposabljanja Degree
Alan Bizjak	V. Vlachy	2005–2010	doktorski študij / *PhD*
Igor Drobnak	A. Jamnik	2006–2011	doktorski študij / *PhD*
Boštjan Jerman	K. Kogej	2004–2008	doktorski študij / *PhD*
Andrej Lajovic	V. Vlachy	2007–2012	doktorski študij / *PhD*
Martin Tine Perger	M. Bešter Rogač	2004–2008	doktorski študij / *PhD*
Mario Šimić	J. Lah	2005–2009	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

Fizikalna kemija / *Physical Chemistry* – UNI in VSŠ
Fizikalna kemija II / *Physical Chemistry II* – UNI
Delovno okolje – prah (aerosoli) / *Working Environment – Aerosols* – VSŠ
Praktikum – uvod v prakso / *Introduction to Practical Work* – VSŠ
Merjenje in regulacija / *Measurements* and *Regulations* – VSŠ
Fizikalna kemija in meritve / *Physical Chemistry and Measurements* – VSŠ
Površinska in koloidna kemija / *Surface and Colloid Chemistry* – UNI
Struktura atomov in molekul / *Structure of Atoms and Molecules* – UNI
Računalništvo in informatika / *Computer Science and Informatics* – VSŠ
Instrumentalne metode / *Instrumental Methods* – UNI
Makromolekulska kemija / *Macromolecular Chemistry* – UNI
Merjenje, regulacija, avtomatizacija / *Measurement, Regulations, Automatisation* – UNI
Biofizikalna kemija / *Biophysical Chemistry* – UNI

Metodika eksperimentov v fizikalni kemiji / *Methodology of Experiments in Physical Chemistry* – UNI

Podiplomski programi / *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

Dodiplomski programi / *Undergraduate Programmes*

Fizikalna kemija / *Physical Chemistry* FFA – UNI in VSŠ

Fizikalna kemija / *Physical Chemistry* NTF – UNI

Fizikalna kemija / *Physical Chemistry* PEF – UNI

Fizikalna kemija / *Physical Chemistry* BF – UNI

Fizikalna kemija II / *Physical Chemistry II* PEF – UNI

Procesna tehnika v živilstvu II / *Process Techniques in Food Technology II* BF – UNI

Vaje iz fizikalne kemije / *Physical Chemistry Laboratory* FMF – UNI

Podiplomski programi / *Postgraduate Programmes*

Koloidna kemija / *Colloid Chemistry* – BF

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 Properies of Different Stereoregular Polyelectrolytes*

Termodinamične in transportne lastnosti raztopin ionenov z različnimi protiioni / *Thermodynamic and 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*

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 lastnosti koloidnih disperzij ter različnih mikroemulzij in gelov / *Research into Structural Properties of Colloid Dispersions, Microemulsions and Gels*

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 / *Modeling 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*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

– A. Lajovic, Prešernova nagrada Univerze v Ljubljani za leto 2007 (mentor A. Jamnik) / *The University Prešeren Award for 2007*
– S. Peljhan, Prešernova nagrada FKKT za leto 2007 (mentorica K. Kogej) / *The Faculty Prešeren Award for 2007*
– G. Trefalt, Prešernova nagrada FKKT za leto 2007 (mentorica B. Hribar Lee) / *The Faculty*

Prešeren Award for 2007

– K. Rade, Prešernova nagrada FKKT za leto 2007 (mentorica K. Kogej) / *The Faculty Prešeren Award for 2007*
– I. Prislan, Krkina nagrada za doktorsko delo v letu 2007 (mentor G. Vesnaver) / *The Krka Award for PhD Thesis in 2007*
– M. Seručnik, Krkina nagrada za diplomsko delo v letu 2007 (mentor J. Lah) / *The Krka Award for BSc Thesis in 2007*
– I. Prislan, 2. nagrada za poster na »*Current Trends in Microcalorimetry Conference*« / *2nd Award for the Best Poster Presentation*, Boston, July 2007.

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

– V. Vlachy (gostujoči urednik / *Guest Editor*), M. Bešter Rogač (gostujoča urednica / *Guest Editor*), *J. Mol. Liq* 2007, vol. 131/132, Amsterdam, Elsevier

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

– C. Pohar (član organizacijskega odbora) / *Member of the Organising Committee*, »European Polymer Congress 2007«, Portorož 2007

DRUGO / OTHER

– K. Kogej, oponent pri zagovoru doktorske disertacije Petra Nilssona, Univerza v Uppsali, Švedska, 2007 / *Opponent at the Defense of Peter Nilsson's Doctoral Disseration, University of Uppsala, Sweden, 2007*
– A. Bizjak, dvomesečno izpopolnjevanje v ZDA v okviru študija mladega raziskovalca / *Two-Month Professional Training of Young Resercher,* USA, 2007
– M. Lukšič: Ad Futura polletna štipendija za doktorski študij 2007 / *Six – Month Ad Futura Fellowship for Doctoral Study*
– M. Tomšič, podoktorski študij na Univerzi v Gradcu, Inštitut za kemijo (prof. O. Glatter) / *Post Doctoral Study, University of Graz, Institute for Chemisty (Prof. O. Glatter),* May 2006 – April 2007
– J. Dolenc, podoktorska štipendija na Zvezni tehniški visoki šoli (ETH) / *Post Doctoral Fellowship at ETH*, Zürich

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

– Diferenčni dinamični kalorimeter N-DSC II (CSC, ZDA) / *Nano II Differential Scanning Calorimter II (CSC, USA)*

- UV-VIS Spektrophotometer Cary BIO 100 (Varian, Avstralija)
- CD Spectrometer 62A DS (Aviv, ZDA)
- Titracijski mikrokalorimeter VP-ITC (Microcal, ZDA) / *Isothermal Titration Microcalorimeter VP-ITC (Microcal, USA)*
- Računalniška gruča iz 20 dvoprocesorskih računalnikov AMD MP 2600+ / *20-Node Cluster Based on Dual AMD MP 2600+ Server CPUs*
- Računalniška gruča iz 8 dvojedrnih 64 bitnih AMD Athlonov 64 X2 4200 / *Eight- Node Computer Cluster Based on Dual AMD Athlon 64 X2 4200+ Server CPUs*
- Sistem za ozkokotno rentgensko sipanje / *Small X-Ray Scattering Instrument*
- Fluorimeter: Luminescence Spectrometer LS 50, Perkin Elmer / *Fluorimeter: Luminescence Spectrometer LS 50, Perkin Elmer*
- Membranski osmometer Knauer / *Membrane Osmometer; Knauer*
- Osmometer na parni tlak: K-7000, Knauer / *Vapour Pressure Osmometer, K-7000 Knauer*
- Sistem za merjenje gostot tekočin DMA 5000, Paar z nihajočo kapilaro prostornine 1 ml / *Vibrating Tube Densimeter, DMA 5000 Paar (1 ml Cell)*
- Titracijski kalorimeter: 2277 Thermal Activity Monitor, ThermoMetric/ *Titration Calorimeter: 227 Thermal Activity Monitor*
- *LKB 10700 (Flow, Batch) Calorimeter*
- Sistem za precizno merjenje električne prevodnosti raztopin (predtermostat Lauda WK 1400, termostat Lauda UB 40 (+/- 0,003 C), LCR Agilent 4284A, DMM Agilent 3458A z uporovnim termometrom Pt100, set različnih celic) / *System for High-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 dinamično sipanje laserske svetlobe 3D DLS, LS Instruments / *Dynamic Light Scattering Instrument 3D DLS, LS Instruments*
- Diferenčni difraktometer DnDc 2010, Brookhaven Instruments / *Differential Diffractometer DnDc 2010, Brookhaven Instruments*
- Gostotomer Paar, DMA 5000 / *Paar Densimeter, DMA 5000*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P1-0201 Fizikalna kemija / *Physical Chemistry*
Vodja programa / *Principal Researcher:* V. Vlachy

TEMELJNI PROJEKTI / BASIC RESEARCH

J1-6653 Lastnosti ionskih raztopin in disperznih sistemov / *Properties of Ionic Solutions and Dispersed Systems*
Nosilec / *Principal Researcher:* V. Vlachy

Z1-9576 Simulacije molekulske dinamike nukleinskih kislin: struktura, dinamika in termodinamska stabilnost / *Molecular Dynamics Simulations of Nucleic Acids: Structure, Dynamics and Thermodynamic Stability*
Nosilec / *Principal Researcher*: J. Dolenc

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

BIO 08/2006 Biofizikalno-kemijska karakterizacija rekombinantnih zdravil / *Biophysicochemical Characterisation of Recombinant Drugs*
Nosilca / *Principal Researchers*: J. Lah, G. Vesnaver
Financer / *Sponsored by:* Lek d.d.

Razvoj in zboljšava tehnologije razžveplevanja dimnih plinov z doziranjem dodatkov v TE Šoštanj / *Development and Improvement of the Flue Gas Desulphurisation Process in TE Šoštanj Using Some Additives*
Nosilec / *Principal Researcher*: J. Golob (sodelavec / *Collaborator* V. Vlachy)
Financer / *Sponsored by*: TE Šoštanj

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

- V. Vlachy, *Statistical Mechanics of Liquids and Solutions,* (zimski semester 2007, predavanja, računske vaje; skupaj s prof. H. Krienkejem), Univerza v Regensburgu, Nemčija / (*Winter Semester 2007, Lectures, Seminars; Together with Prof. Krienke*), *University of Regensburg, Germany*
- V. Vlachy, gostujoči profesor, Univerza v Regensburgu / *Visiting Professor, University of Regensburg,* 15. 10. 2006–14. 4. 2007
- V. Vlachy, gostujoči profesor, Univerza Pierre in Marie Curie, Pariz / *Visiting Professor, University Pierre&Marie Curie, Paris,* 15. 5.–15. 6. 2007
- A. Godec, mentor slovenske srednješolske ekipe na mednarodni kemijski olimpiadi v Moskvi / *Mentor of the Slovenian Team on International Chemistry Olympiad, Moscow,* 2007
- J. Dolenc, asistentka na Zvezni tehniški visoki šoli (ETH), Zürich, pri prof. dr. W. F. van Gunsternu 2006–2008 / *Teaching Assistant at the ETH, Zürich (Prof. W.G. van Gunstern),* 2006–2008

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL SCIENTIFIC COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

COST D–31	*Organising Noncovalent Chemical Systems with Selected Functions* Nosilec / *Principal Researcher*: G. Vesnaver
COST D–43	*Colloid and Interface Chemistry for Nanotechnology* Nosilec / *Principal Researcher*: M. Bešter Rogač

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Avstrija *Slovenia – Austria*	Nanostrukturirane kompleksne raztopine – struktura in kinetika v novih materialih / *Nanostructured Complex Fluids – Structure and Kinetics in New Materials* Nosilec / *Principal Researcher:* A. Jamnik
Slovenija – Francija (Proteus) *Slovenia – France (Proteus)*	Uporaba Brownovske dinamike za študij sistemov z delno »zamrznjenimi« prostostnimi stopnjami / *Brownian Dynamic Study of Partly Quenched Systems* Nosilec / *Principal Researcher*: V. Vlachy
Slovenija – ZDA *Slovenia – USA*	Vpliv dodatka linearnega polielektrolita na hitrost kemijske reakcije med ioni / *Influence of the Addition of Linear Polyelectrolyte on the Reaction Rate Between Low – Molecular Ions* Nosilec / *Principal Researcher*: V. Vlachy
Slovenija – Ukrajina *Slovenia – Ukraine*	Hidratacija enostavnih in verigastih molekul; 2. Raztopine polielektrolitov / *Hydration of Simple and Chain-Like Molecules; 2. Polyelectrolyte Solutions* Nosilec / *Principal Researcher:* V. Vlachy
Slovenija – ZDA *Slovenia – USA*	Voda ob kompleksnih površinah / *Water Near Complex Surfaces* Nosilec / *Principal Researcher*: B. Hribar Lee
Slovenija – ZDA (NIH) *Slovenia – USA (NIH Grant)*	Modeliranje hidratacije v biologiji / *Modelling Hydration in Biology* Nosilca / *Principal Researchers:*: V. Vlachy, K.A. Dill (UC San Francisco)

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

- K. Kogej, *Isotactic Versus Atactic Poly(Methacyclic Acid): Solution Behaviour and Interaction with Surface Active and Simple Counterions*, Department of Pharmacy, University of Uppsala, Uppsala, Sweden, October 2007
- K. Kogej, *Polyelectrolyte–Surfactant Interactions*, Department of Pharmacy, University of Uppsala, Uppsala, Sweden, October 2007
- M. Bešter Rogač, *Pharmaceutically Applicable Surfactant System: A Challenge for the Physical Chemist,* Departament de Technologia de Tensioactius, Institut d'Investigaciones Químiques i Ambientals de Barcelona (IIQAB), Barcelona, Spain, June 2007
- T. Urbič, *Three-State Model of Water*, Department of Pharmaceutical Chemistry and Graduate Group in Biophysics, University of California, San Francisco, USA, September 2007
- Č. Podlipnik, *Two Strategies for the Design of Prophylactic Cures Against Cholera*, Università degli Studi di Milano, Milano, Italy, May 2007
- V. Vlachy, vabljeno predavanje, *Polyelectrolyte Hydration: Theory and Experiment*, 30th International Conference on Solution Chemistry, Perth, Australia, July 2007
- V. Vlachy, *Polyelectrolyte Hydration: Experiment, Theory, and Simulation*, Centre de Recherche sur l'Energie Nucléaire (CEA), Saclay, France, May 2007
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Maja Harej	D. Dolenc	2003–2007	doktorski študij / *PhD*
Ana Bergant	J. Cerkovnik	2004–2009	doktorski študij / *PhD*
Vita Majce	S. Polanc	2007–2012	doktorski študij / *PhD*
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Jure Hren	M. Kočevar	2006–2010	doktorski študij / *PhD*
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Gaj Stavber	M. Zupan	2005–2009	doktorski študij / *PhD*
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Uroš Uršič	B. Stanovnik	2004–2009	doktorski študij / *PhD*
Jernej Wagger	B. Stanovnik	2005–2008	doktorski študij / *PhD*

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Organska kemija / *Organic Chemistry* – VSŠ
Organska kemija II / *Organic Chemistry II* – UNI
Organska analiza / *Organic Analysis* – UNI

Splošna kemija II / *General Chemistry II* – VSŠ

Spektroskopske metode / *Spectroscopic Methods* – UNI

Analitika in spektroskopija / *Analysis and Spectroscopy* – VSŠ

Kemija heterocikličnih spojin / *Chemisty of Heterocyclic Compounds* – UNI

Načrtovanje organskih sintez / *Planning of Organic Syntheses* – UNI

Izbrana poglavja iz organske kemije / *Selected Topics in Organic Chemistry* – UNI

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Pretvorbe bioaktivnih spojin / *Transformations of Bioactive Compounds* – UNI

Nukleinske kisline in polinukleotidi / *Nucleic Acids and Polynucleotides* – UNI

Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UNI

Poskusi v organski kemiji / *Experiments in Organic Chemistry* – UNI

Podiplomski programi / *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 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

Dodiplomski programi / *Undergraduate Programmes*

Kemija / *Chemistry* PEF – UNI

Kemija II / *Chemistry II* NTF – VSŠ

Organska kemija / *Organic Chemistry* FFA – UNI in VSŠ
Organska kemija / *Organic Chemistry* NTF – UNI in VSŠ
Organska kemija / *Organic Chemistry* PEF – UNI
Organska kemija / *Organic Chemistry* BF – UNI
Kemija organskih materialov / *Chemistry of Organic Materials* NTF – UNI
Teoretske osnove tiskarskih procesov / *Fundamental Theoretical Principles of Printing Processes* NTF – UNI

Podiplomski programi (UPŠ Biomedicina) / *Postgraduate Programmes (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*
- Kombinatorna in paralelna sinteza / *Combinatorial and Parallel Synthesis*
- 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*
- Sinteza in uporaba novih ligandov za asimetrično heterogeno katalizo / *Synthesis and Application of New Ligands for Asymmetric Heterogeneous Catalysis*
- 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*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

– P. Čebašek D. Bevk, S. Pirc, B. Stanovnik, J. Svete:
Nagrada American Chemical Society za najbolj citiran članek v reviji Journal of Combinatorial Chemistry v letu 2006; "Parallel Synthesis of 3-Amino-4*H*-Quinolizin-4-ones, Fused 3-Amino-4*H*-Pyrimidin-4-ones, and Fused 3-Amino-2*H*-Pyran-2-ones", objavljen v reviji *Journal of Combinatorial Chemistry*, **2006**, *8*, 95–102.
The American Chemical Society nominated this article as the most cited article in the Journal of Combinatorial Chemistry in 2006.

– U. Grošelj, D. Bevk, R. Jakše, A. Meden, S. Pirc, S. Rečnik, B. Stanovnik, J. Svete:
Nagrada založniške hiše Elsevier Ltd. za najbolj citiran članek v reviji Tetrahedron:Asymmetry v letih 2004–2007; "Synthesis and properties of N-substituted (1*R*,5*S*)-4-aminomethylidene-1,8,8-trimethyl-2-oxabicyclo[3.2.1]octan-2-ones", objavljen v reviji *Tetrahedron:Asymmetry*, **2004**, *15*, 2367–2383.
The Elsevier Ltd. nominated this article as the most cited article in Tetrahedron: Asymmetry in the period from 2004 to 2007.

– B. Stanovnik:
Diploma in medalja *"In Memory of Professor A. N. Kost"* za dosežke v kemiji heterocikličnih spojin za leto 2007, ki jo podeljujejo International Scientific Partnership Foundation, Lomonosov Moscow State University and Mendeleev Russian Chemical Society.
Diploma and medal "In Memory of Professor A. N. Kost" *for the achievements in the chemistry of heterocyclic compounds for the year 2007, awarded by the International Scientific Partnership Foundation, Lomonosov Moscow State University and Mendeleev Russian Chemical Society.*

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*

DRUGO / OTHER

– M. Kočevar je postal Nacionalni predstavnik v odboru (komiteju) Organic and Biomolecular Chemistry Division (III) IUPAC (za leti 2008–2009) / *Appointed as a National Representative, IUPAC Organic and Biomolecular Division (III) Committee for the Period 2008–2009*

– F. Požgan je bil na podoktorskem izobraževanju v Franciji v okviru Evropskega programa Marie Curie Grant / *Postdoctoral Fellowship, Marie Curie Grant*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- C, H, N – Analizator Perkin-Elmer 2400 II / *C, H, N – Analyzer Perkin Elmer 2400 II*
- UV – visible spektrofotometer Varian / *UV – Visible Spectrophotometer Varian*
- IR spektrometer BIO-RAD / *IR Spectrometer BIO-RAD*
- IR spektrometer Spectrum BX FTIR Perkin-Elmer / *IR Spectrometer Spectrum BX FTIR Perkin-Elmer*
- Polarimeter Perkin-Elmer / *Polarimeter Perkin-Elmer*
- Destilacijska aparatura Fisher-Jones / *Distillation Apparatus Fisher-Jones*
- Mettler-Toledo miniblock paralelni sintetizator – 12 pozicij / *Mettler-Toledo Miniblock Parallel Synthesizer – 12 Positions*
- Carousel reaction station paralelni sintetizator – 6 pozicij / *Carousel Reaction Station Paralel Synthesizer – 6 Positions*
- Büchi Syncore Polyvap+Reactor paralelni sintetizator in uparjevalnik– 24 pozicij / *Büchi Syncore Polyvap+Reactor Parallel Syntesizer and Evaporator – 24 Positions*
- 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 °C / *Cooler –60 °C*
- Hidrogenator Parr / *Parr Hydrogenator*
- Avtoklavi Berghof / *Autoclaves Berghof*
- Rotavaporji Büchi / *Rotavapors Büchi*

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*
Nosilec / *Principal Researcher:* B. Stanovnik

P1-0230 Organska kemija: Sinteza, struktura in aplikacija / *Organic Chemistry: Synthesis, Structure, and Application*
Nosilec / *Principal Researcher:* M. Kočevar

TEMELJNI PROJEKTI / BASIC RESEARCH

J1-6254 Reaktivni intermediati pri transformacijah organskih spojin / *Reactive Intermediates in the Transformation of Organic Compounds*
Nosilec / *Principal Researcher:* B. Plesničar

J1-6693 Od multifunkcionalnih gradnikov do biološko aktivnih spojin / *From Multifunctional Building Blocs to Biologically Active Compounds*
Nosilec / *Principal Researcher:* M. Kočevar

J1-6689 Sinteza heterocikličnih analogov aminokislin in peptidov / *Synthesis of Heterocyclic Analogs of Amino Acids and Peptides*
Nosilec / *Principal Researcher:* B. Stanovnik

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

CRO-S 16 / 2006 Optimizacija postopka sinteze hipolipidemika / *Optimization of the Synthesis of a Hypolipidemic Agent*
Nosilec / *Principal Researcher:* J. Košmrlj
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* M. Kočevar
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* B. Stanovnik
Financer / *Sponsored by:* Lek d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* B. Stanovnik
Financer / *Sponsored by:* Krka d.d.

Donacija za nakup opreme / *Donation for Purchasing the Equipment*

Nosilec / *Principal Researcher:* B. Stanovnik
Donator / *Donated by:* Krka d.d.

Pogodba o sodelovanju / *Cooperation Agreement*
Nosilec / *Principal Researcher:* J. Svete
Financer / *Sponsored by:* Boehringer-Ingelheim Pharma, Biberach, Nemčija

Donacija opreme / *Donation of Equipment*
Nosilec / *Principal Researcher:* J. Svete
Donator / *Donated by:* Boehringer-Ingelheim Pharma, Biberach, Nemčija

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

COST D24/0007/02	*Synthesis and Application of New Ligands for Asymmetric Heterogeneous Catalysis* Nosilec / *Principal Researcher*: M. Kočevar

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Kitajska *Slovenia – China*	Študij novih reakcij izomerno čistih α,β-didehidroaminokislinskih derivatov / *Studies of New Reactions of Isomerically-Pure α,β-Didehydroamino Acid Derivatives* Nosilec / *Principal Researcher*: M. Kočevar
Slovenija – Hrvaška *Slovenia – Croatia*	Sinteza in evalvacija novih potencialnih citostatikov diazenskega tipa / *Synthesis and Evaluation of New Potential Cytostatics from Diazenes Family* Nosilec / *Principal Researcher*: S. Polanc
Slovenija – Hrvaška *Slovenia – Croatia*	Elektronska struktura halogeniranih difenilmetanonov in difeniletanonov / *Electronic Structure of Halogenated Diphenilmethanones and Diphenilethanones* Nosilec / *Principal Researcher*: B. Šket
Slovenija – Češka *Slovenia – Czech Republic*	Sinteza in premestitve nekaterih prikondenziranih kinolonov / *Synthesis and Molecular Rearrangements of Some Fused Quinolones* Nosilec / *Principal Researcher*: J. Košmrlj
Slovenija – Češka *Slovenia – Czech Republic*	Nov pristop k antibakterijsko aktivnim molekulam / *New Approach to Antibacterial Active Molecules* Nosilec / *Principal Researcher:* S. Polanc

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

- M. Kočevar, *2H-Pyran-2-Ones and Fused Pyran-2-Ones as Versatile Tools in Organic Synthesis,* Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, June 2007
- S. Polanc, *Recent Advances in the Chemistry of Nitrogen-Chain Compounds,* College of Life Sciences, China Jiliang University, Hangzhou, China, June 2007
- S. Polanc, *Synthetic Potential of Selected Nitrogen-Containing Compounds,* Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, October 2007
- S. Polanc, *Synthetically Useful Products Obtained from Diazenes, Triazenes and Some Other Compounds,* Faculty of Pharmacy, Charles University, Hradec Kralove, Czech Republic, October 2007
- J. Svete, *Enaminones: Versatile Reagents in the Combinatorial Synthesis of Heterocycles,* Boehringer-Ingelheim Pharma, Biberach, Germany, September 2007
- J. Svete, *Recent Applications of Enaminones and Azomethine Imines in Combinatorial Synthesis of Heterocycles,* University of Jena, Jena, Germany, September 2007

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

- Prof. Dr. Peter Langner, Institut für Chemie, Abteilung Organische Chemie, Universität Rostock, Rostock, Germany, *Synthesis of Carbo- and Heterocycles by One-Pot Cyclizations of Free and Masked Dianions,* June 2007
- Prof. Dr. Dieter Seebach, Laboratorium für Organische Chemie, ETH, Hönggerberg, Zürich, Switzerland, *Organocatalysis – Alternative Old and New Contributions to View at the Mechanism of Proline-Catalyzed Reactions,* May 2007
- Prof. Dr. Sergey Vasilevsky, Institute of Chemical Kinetics & Combustion, Russian Academy of Sciences, Sibirian Branch, Novosibirsk, Russia, *Cyclization of Vic-Functionalized Aryl(hetaryl)alkynes. Effective Strategy for the Synthesis of Condensed Heterocycles*, June 2007

BIBLIOGRAFIJA 2007 / REFERENCES 2007

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

OK1. POŽGAN, Franc, KRANJC, Krištof, KEPE, Vladimir, POLANC, Slovenko, KOČEVAR, Marijan. Synthesis of 2H-pyran-2-ones and fused pyran-2-ones as useful building blocks. *ARKIVOC*. [Print ed.], 2007, vol. VIII, str. 97-111, Graf. prikazi. [COBISS.SI-ID 28282885]

OK2. KOVAČ, Andreja, MAJCE, Vita, LENARŠIČ, Roman, BOMBEK, Sergeja, BOSTOCK, Julieanne, CHOPRA, Ian, POLANC, Slovenko, GOBEC, Stanislav. Diazenedicarboxamides as inhibitors of D-alanine-D-alanine ligase (Ddl). *Bioorg. med. chem. lett.*. [Print ed.], 2007, vol. 17, no. 7, str. 2047-2054. [COBISS.SI-ID 2063985]

OK3. IMRAMOVSKÝ, Aleš, POLANC, Slovenko, VINŠOVÁ, Jarmila, KOČEVAR, Marijan, JAMPÍLEK, Josef, REČKOVÁ, Zuzana, KAUSTOVÁ, Jarmila. A new modification of anti-tubercular active molecules. *Bioorg. med. chem.*. [Print ed.], 2007, vol. 15, no. 7, str. 2551-2559, graf. prikazi. [COBISS.SI-ID 28453637]

OK4. KRANJC, Krištof, KOČEVAR, Marijan. Enhancing a neat microwave-assisted transformation. Diels-Alder reaction of 2H-pyran-2-ones toward fused bicyclo[2.2.2]octenes. *Bull. Chem. Soc. Jpn.*, 2007, vol. 80, no. 10, str. 2001-2007. [COBISS.SI-ID 28996101]

OK5. JEREB, Marjan, TOGNI, Antonio. Ti[sup](IV)-catalyzed asymmetric sulfenylation of 1,3-dicarbonyl compounds. *Chemistry (Weinh., Print)*. [Print ed.], 2007, vol. 13, no. 33, str. 9384-9392. [COBISS.SI-ID 29126149]

OK6. KRIŽMAN LAVRIČ, Pavla, KOVAČ, Franci, FORTE-TAVČER, Petra, HAUSER, Peter J., HINKS, David. Enhanced PAA bleaching of cotton by incorporating a cationic bleach activator. *Color. technol.*, 2007, vol. 123, no. 4, str. 230-236. [COBISS.SI-ID 1826160]

OK7. PODGORŠEK, Ajda, STAVBER, Stojan, ZUPAN, Marko, ISKRA, Jernej. Bromination of ketones with H[sub]2O[sub]2-HBr "on water". *Green chem. (Print)*, 2007, issue 11, vol. 9, str. 1212-1218. [COBISS.SI-ID 21186343]

OK8. BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, SVETE, Jurij, STANOVNIK, Branko. Synthesis and transformation of methyl 2-(6-hydroxy-2-phenyl-pyrimidin-4-yl)acetate : simple preparation of pyrimidines with heterocyclic substituents. *Helv. Chim. Acta*, 2007, vol. 90, no. 9, str. 1737-1744, graf. prikazi. [COBISS.SI-ID 28919813]

OK9. BEVK, David, SVETE, Jurij, STANOVNIK, Branko. Synthesis of 2-unsubstituted 2,3,5,6,7,8-hexahydropyrazolo[4,3-d][1, 2]diazepinone-8-carboxylates. *Heterocycles*, 2007, vol. 71, no. 3, str. 657-668, graf. prikazi. [COBISS.SI-ID 28448773]

OK10. HREN, Jure, KRANJC, Krištof, POLANC, Slovenko, KOČEVAR, Marijan. Bicyclo[2.2.2]oct-7-ene derivatives : a green preparation of the fused succinimide ring. *Heterocycles*, 2007, vol. 72, no. 1, str. 399-410. [COBISS.SI-ID 28571397]

OK11. KRANJC, Krištof, KOČEVAR, Marijan. Microwave-assisted Diels-Alder reaction of 2H-pyran-2-ones with maleimides towards fused bicyclo[2.2.2]octenes. *Heterocycles*, 2007, vol. 73, no. 1, str. 481-491. [COBISS.SI-ID 29139973]

OK12. JAKŠE, Renata, GROŠELJ, Uroš, SORŠAK, Gorazd, SVETE, Jurij, STANOVNIK, Branko. Synthesis of thioaplysinopsin analogs derived from 5-dimethylaminomethylidene-2-thioxo-1,3-thiazol-4-ones. *Heterocycles*, 2007, vol. 73, no. 1, str. 743-750. [COBISS.SI-ID 29139461]

OK13. MODEC, Barbara, DOLENC, Darko, BRENČIČ, Jurij. New molybdenum(V) complexes based on the {M o[sub]2O[sub]4}[sup](2+) structural core with esters or anions of malonic and succinic acid. *Inorg. Chim. Acta*. [Print ed.], 2007, vol. 360, no. 2, str. 663-678, graf. prikazi. [COBISS.SI-ID 28869637]

OK14. CERAR, Janez, POMPE, Matevž, GUČEK, Marjan, CERKOVNIK, Janez, ŠKERJANC, Jože. Analysis of sample of highly water-soluble T[sub]-symmetric fullerenehexamalonic acid C[sub](66)(COOH)[sub](12) by ion-chromatography and capillary electrophoresis. *J. chromatogr.*, 2007, vol. 1169, no. 1/2, str. 86-94. [COBISS.SI-ID 28975365]

OK15. MALAVAŠIČ, Črt, BRULC, Blaž, ČEBAŠEK, Petra, DAHMANN, Georg, HEINE, Niklas, BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Combinatorial solution-phase synthesis of (2S,4S)-4-acylamino-5-oxopyrrolidine-2-carboxamides. *J. comb. chem.*, 2007, vol. 9, no. 2, str. 219-229. [COBISS.SI-ID 28465925]

OK16. PEZDIRC, Lidija, BEVK, David, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Combinatorial solution-phase synthesis of alkyl (1S*,2S*,3R*,5R*,6R*)-1-alkyl-3-aryl-6-benzoylamino-1-hydroxy-7- oxo-5-phenylhexahydropyrazolo[1, 2-a]pyrazole-2-carboxylates. *J. comb. chem.*, 2007, vol. 9, no. 4, str. 717-723. [COBISS.SI-ID 28752389]

OK17. IOSIF, Florentina, PARVULESCU, Vasile I., PEREZ-BERNAL, M. Elena, RUANO-CASERO, Ricardo J., RIVES, Vicente, KRANJC, Krištof, POLANC, Slovenko, KOČEVAR, Marijan, GENIN, Emilie, GENÊT, Jean-Pierre, MICHELET, Véronique. Heterogeneous hydrogenation of bicyclo[2.2.2]octenes on Rh/TPPTS/LDH catalysts. *J. mol. catal., A Chem.*, 2007, vol. 276, no. 1/2, str. 34-40, graf. prikazi. [COBISS.SI-ID 28857861]

OK18. HAREJ, Maja, DOLENC, Darko. Autoxidation of hydrazones. Some new insights. *J. org. chem.*, 2007, vol. 72, no. 19, str. 7214-7221, graf. prikazi. [COBISS.SI-ID 28871685]

OK19. ŽMITEK, Katja, ZUPAN, Marko, STAVBER, Stojan, ISKRA, Jernej. The effect of iodine on the peroxidation of carbonyl compounds. *J. org. chem.*, 2007, vol. 72, str. 6534-6540. [COBISS.SI-ID 20969511]

OK20. BOUDEBOUS, Hassen, KOŠMRLJ, Berta, ŠKET, Boris, WIRZ, Jakob. Primary photoreactions of the 3,5-dimethoxybenzoin cage and determination of the release rate in polar media. *J. phys. chem., A Mol. spectrosc. kinet. environ. gen. theory*, 2007, vol. 111, no. 15, str. 2811-2813, graf. prikazi. [COBISS.SI-ID 28844549]

OK21. KOŠMRLJ, Janez, KAFKA, Stanislav, LEBAN, Ivan, GRAD, Mateja. Formation and structure elucidation of two novel spiro[2H-indol]-3(1H)-ones. *Magn. reson. chem.*, 2007, vol. 45, no. 8, str. 700-704, ilustr. [COBISS.SI-ID 28716805]

OK22. LIU, Jie, KEPE, Vladimir, ŽABJEK, Alenka, PETRIČ, Andrej, PADGETT, Henry C., SATYAMURTHY, Nagichettiar, BARRIO, Jorge R. High-yield, automated radiosynthesis of 2-(1-{6-[(2-[[sup](18)F]fluoroeth yl)(methyl) amino]-2-naphthyl}ethylidene)malononitrile ([[sup](18)F]FDDNP) ready for animal or human administration. *Mol. imaging biol.*, 2007, vol. 9, no. 1, str. 6-16, graf. prikazi. [COBISS.SI-ID 28414725]

OK23. ŽMITEK, Katja, ZUPAN, Marko, ISKRA, Jernej. [Alpha]-substituted organic peroxides: synthetic strategies for a biologically important class of gem-dihydroperoxide and perketal derivatives. *Organic and Biomolecular Chemistry*. [Print ed.], 2007, vol. 5, no. 24, str. 3895-3908. [COBISS.SI-ID 21293607]

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OK32. WAGGER, Jernej, GOLIČ GRDADOLNIK, Simona, GROŠELJ, Uroš, MEDEN, Anton, STANOVNIK, Branko, SVETE, Jurij. Chiral solvating properties of (S)-1-benzyl-6-methylpiperazine-2,5-dione. *Tetrahedron: asymmetry*. [Print ed.], 2007, vol. 18, no. 4, str. 464-475, ilustr. [COBISS.SI-ID 28478981]

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OK38. STAVBER, Gaj. The use of molecular oxygen in organic synthesis. *Synlett*, 2007, no. 20, str. 3224-3225. http://dx.doi.org/DOI:10.1055/s-2007-990887. [COBISS.SI-ID 21286951]

KRATKI ZNANSTVENI PRISPEVEK / SHORT SCIENTIFIC ARTICLE

OK39. STAVBER, Gaj, ZUPAN, Marko, STAVBER, Stojan. Solvent-free fluorination of organic compounds using N-F reagents. *Tetrahedron lett.*. [Print ed.], 2007, vol. 48, str. 2671-2673. [COBISS.SI-ID 20625703]

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

OK40. STANOVNIK, Branko. [Beta]-dimethylamino-[alpha],[beta]-didehydro-[alpha]-amino acid derivatives and related compounds in the synthesis. Preparation of various heterocyclic systems including natural products : [invited lecture]. V: *10th Ibn sina international conference on pure and applied heterocyclic chemistry, [10th ISIC], Isis hotel, Luxor-Egypt, february 17-20, 2007 : abstracts*. [S. l.: s. n.], 2007, str. 17-18, ilustr. [COBISS.SI-ID 28475909]

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OK49. POŽGAN, Franc, DIXNEUF, Pierre H. Recent applications of alkene metathesis for fine chemicals and supramolecular system synthesis. V: İMAMOGLU, Yavuz (ur.), DRAGUTAN, Valerian (ur.). *Metathesis chemistry : from nanostructure design to synthesis of advanced materials : proceedings of the NATO Advanced Study Institute on New Frontiers in Technologies for Synthesis of Advanced Materials, Antalya, Turkey, 4-16 September 2006*, (NATO science series, Series II,, Mathematics, physics, and chemistry, Vol. 243). Dordrecht; London: Springer, 2007, str. 195-222. [COBISS.SI-ID 29160709]

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OK51. POLANC, Slovenko, STANOVNIK, Branko. *Določevanje strukture organskih spojin s spektroskopskimi metodami*. [1. ponatis]. Ljubljana: Fakulteta za naravoslovje in tehnologijo, Oddelek za kemijo, 1986. 2 zv. [COBISS.SI-ID 17937664]

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

OK52. GLAŽAR, Saša A., GRAUNAR, Mojca, MODEC, Barbara, ŠKET, Barbara, ŠKET, Boris. *Kemija danes : učenje z nalogami : zbirka nalog za 8. in 9. razred devetletne osnovne šole*, (Raziskovalec 8), (Raziskovalec 9). 1. izd. Ljubljana: DZS, 2007. 184 str., ilustr. ISBN 978-86-341-3645-6. [COBISS.SI-ID 231367168]

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OK53. DOLENC, Darko, MODEC, Barbara. *Kemija za devetletko : zbirka testnih nalog za 8. in 9. razred devetletne osnovne šole*. 1. izd. Ljubljana: DZS, 2007. 64 str., ilustr. ISBN 978-86-341-4207-5. [COBISS.SI-ID 231737088]

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PATENTNA PRIJAVA / PATENT APPLICATION

OK59. GOBEC, Stanislav, KOVAČ, Andreja, BRAJIĆ, Alja, PEČAR, Slavko, BOSTOCK, Julieanne, CHOPRA, Ian, LENARŠIČ, Roman, BOMBEK, Sergeja, KOČEVAR, Marijan, POLANC, Slovenko. *Diazenedicarboxamides as inhibitors of D-alanine: D-alanine ligaes (Ddl) : European patent no. EP07468010, publication date: 07. avgust 2007. Munich: European Patent Organisation, 2007*. [COBISS.SI-ID 2166129]

OK60. ANDERS, Manfred, LICHTBLAU, Dirk Andreas, KOLAR, Jana, MALEŠIČ, Jasna, STRLIČ, Matija, ŠALA, Martin, KOČEVAR, Marijan. *Antioxidant for an organic material and method for treating the same : US2007/187650 A1*. Leipzig: ZFB Zentrum fur Bucherhaltung, 16.8.2007. 14 str., Ilustr. [COBISS.SI-ID 26939909]

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OK61. KOČEVAR, Marijan. *2H-Pyran-2-ones and fused pyran-2-ones as versatile tools in organic synthesis : [Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 8. 6. 2007]*. Prague, 2007. [COBISS.SI-ID 28691973]

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OK63. POLANC, Slovenko. *Nitrogen-chain compounds: chemistry and biological potential : [Ruđer Bošković Institute, Zagreb, Croatia, november 14, 2007]*. Zagreb, 2007. [COBISS.SI-ID 29087493]

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OK65. SVETE, Jurij. *Recent applications of enaminones and azomethine imines in combinatorial synthesis of heterocycles : [University of Jena, Jena, Germany, 14.9.2007]*. Jena, 2007. [COBISS.SI-ID 28940805]

OK66. POLANC, Slovenko. *Synthetic potential of selected nitrogen-containing compounds : [Institute of Organic Chemistry and Biochemistry, Academy of sciences of the Czech Republic, Prague, October 5, 2007]*. Prague, 2007. [COBISS.SI-ID 28980229]

OK67. POLANC, Slovenko. *Synthetically useful products obtained from diazenes, triazenes and some other compounds : [Faculty of Pharmacy, Charles University, Hradec Kralove, Czech Republic, October 4, 2007]*. Hradec Kralove, 2007. [COBISS.SI-ID 28980485]

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OK68. *Acta chimica slovenica*. Kranjc, Krištof (član uredniškega sveta 2007-). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993-. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]

OK69. DEMŠAR, Alojz, KOČEVAR, Marijan (član ur. odbora), PAVKO, Aleksander, KOCJAN-BARLE, Marta (ur.), BAJT, Drago (ur.), OGRIZEK, Maja (ur.), MOŠKRIČ, Marica (ur.), ALIČ, Snežna (ur.). *Slovenski veliki leksikon*. 1. izd. Ljubljana: Mladinska knjiga, 2007. 12 zv., ilustr. ISBN 978-86-11-17850-9. ISBN 86-11-17850-5. ISBN 978-86-11-17851-6. ISBN 978-86-11-17852-3. ISBN 978-86-11-17853-0. ISBN 978-86-11-17854-7. ISBN 86-11-17854-8. ISBN 978-86-11-17855-4. ISBN 86-11-17855-6. ISBN 978-86-11-17856-1. ISBN 86-11-17856-4. ISBN 978-86-11-17857-8. ISBN 86-11-17857-2. ISBN 978-86-11-17858-5. ISBN 86-11-17858-0. ISBN 978-86-11-17859-2. ISBN 978-86-11-17860-8. ISBN 978-86-11-17861-5. [COBISS.SI-ID 230085888]

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Mladi raziskovalci Young Researchers	Mentor Mentor	Čas usposabljanja Programme Duration	Oblika usposabljanja Degree
Tanja Razpotnik	J. Maček	2003–2007	doktorski študij / *PhD*
Jana Kemperl	J. Maček	2007–2011	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

Gradiva / *Materials* – UNI

Anorganski materiali in produkti,Tehnična keramika in silikati / *Inorganic Materials and Products, Technical Ceramics and Silicates* – UNI

Materiali / *Materials* – VSŠ

Anorganski procesi in produkti / *Inorganic Processes and Products* – VSŠ

Osnove kemijskih tehnoloških procesov / *Fundamentals of Chemical Processes* – UNI

Anorganska kemijska tehnologija / *Inorganic Chemical Technology* – UNI

Pregled tehnologij / *Principles of Technological Processes* – UNI

Uvod v tehnologijo / *Introduction to Technology* – VSŠ

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

Nevarne snovi / *Hazardous Substances* – VSŠ

Podiplomski programi / *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

Dodiplomski programi / *Undergraduate Programmes*

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Industrijski materiali / *Industrial Materials* FMF – UNI

Keramika I / *Ceramics I* NTF – UNI

Gradiva / *Materials* FGG – UNI in VSŠ

Tehnologija kovin in keramike / *Technology of Metals and Ceramics* ALUO – UNI

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 Prep-*

aration; 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 Development for 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

- S. Glinšek, Prešernova nagrada FKKT za leto 2007 (mentor S. Pejovnik) / *The Faculty Prešeren Award for 2007*
- A. Kljajić, Prešernova nagrada FKKT za leto 2007 (mentor S. Pejovnik) / *The Faculty Prešeren Award for 2007*
- P. Podberščček, Prešernova nagrada FKKT za leto 2007 (mentor J. Maček) / *The Faculty Prešeren Award for 2007*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Netzsch STA 409 aparatura za simultano termično analizo */ Apparatus for Simultaneous Thermal Analysis*

- Mettler TA 4000: DSC 20 modul / *DSC 20 Module*
  TG 50 modul / *TG 50 Module*
- Leybold Heraeus Inficon Quadrex QMS-200, masni spektrometer / *Quadrupole Mass Spectrometer*
- 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*
Vodja programa / *Principal Researcher*: I. Leban

TEMELJNI PROJEKTI / BASIC RESEARCH

Z2-7353 Priprava in karakterizacija novih potencialno uporabnih snovi nanometrskih dimenzij s kemijsko transportno reakcijo / *Synthesis and Characterization of New-Potentially Applicable Materials of Nanometer Dimensions with Chemical Transport Reaction*
Nosilec / *Principal Researcher*: D. Vrbanić

J2-6027 Priprava in karakterizacija kompozitnih uniformnih delcev / *Preparation and Characterisation of Uniform Composite Particles*
Nosilec / *Principal Researcher*: Z. Crnjak Orel (KI)

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L2-6471 Razvoj metodologij za oceno tveganj v cestnih predorih / *Development of Methodologies for Risk Analysis of Road Tunnels*
Nosilec / *Principal Researcher*: S. Petelin (UL FPP)
Sofinancer / *Co-sponsored by*: DARS – Družba za avtoceste v RS

M2-0101 Sistem gorivnih celic kot pomožni vir energije za zagotavljanje avtonomnosti vojaških vozil / *Fuel Cell System as an Auxiliary Energy Source for Military Vehicles*
Nosilec / *Principal Researcher*: J. Tavčar (TECES Maribor)
Sofinancer / *Co-sponsored by*: Ministrstvo za obrambo RS

M2-0112 Nadgradnja lahkih kolesnih oklepnih vozil VALUK 6x6 za izvajanje nalog RKB / *Adaptation of Lightly Armored Vehicles Valuk 6x6 for NBC Duties*
Nosilec / *Principal Researcher*: R. Kunc (UL FS)
Sofinancer / *Co-sponsored by*: Ministrstvo za obrambo RS

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VEČSTRANSKO MEDNARODNO SODELOVANJE / MULTILATERAL COOPERATION

BioCellus EU 6. OP *Biomass Fuel Cell Utility System*
Nosilec / *Principal Researcher*: J. Maček

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

- R. Dominko, S. Pejovnik, *Electrochemical Wiring in Battery Materials,* International Battery Materials Association 2007 Conference, Shenzhen, China, November 2007
- S. Pejovnik, *Designing of Electrode Properties in Li Ion Batteries*, Institute of Chemistry, Universidade Estadual Paulista, Araraquara, Brazil, February 2007

BIBLIOGRAFIJA 2007 / REFERENCES 2007

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

ATM1. PODMILJŠAK, Benjamin, MCGUINESS, Paul J., ŽUŽEK ROŽMAN, Kristina, NOVOSEL, Barbara, PEJOVNIK, Stane, KOBE, Spomenka. The effects of nitriding on the magnetic properties of Sm-Fe- and Sm-Fe-Ta-based materials. *J. alloys compd.*. [Print ed.], 2007, vol. 433, str. 256-260. [COBISS.SI-ID 20638759]

ATM2. VRBANIĆ, Daniel, MEDEN, Anton, NOVOSEL, Barbara, PEJOVNIK, Stane, UMEK, Polona, PONIKVAR, Maja, MIHAILOVIĆ, Dragan. Synthesis and characterization of Mo[sub]6S[sub](4.5)I[sub](4.5) nanowires. *J. nanosci. nanotechnol. (Print)*, 2007, vol. 7, no. 3, str. 982-985, Graf. prikazi. [COBISS.SI-ID 28263685]

ATM3. MARINŠEK, Marjan, PADEŽNIK GOMILŠEK, Jana, ARČON, Iztok, ČEH, Miran, KODRE, Alojz, MAČEK, Marijan. Structure development of NiO-YSZ oxide mixtures in simulated citrate-nitrate combustion synthesis. *J. Am. Ceram. Soc.*, 2007, 90, str. 3274-3281. [COBISS.SI-ID 20963623]

ATM4. CRNJAK OREL, Zorica, MAČEK, Jadran, MARINŠEK, Marjan, PEJOVNIK, Stane. Coprecipitation of copper/zinc compounds in metal salt-urea-water system. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, no. 2/3, str. 451-455. [COBISS.SI-ID 3588890]

ATM5. MAČEK, Jadran, NOVOSEL, Barbara, MARINŠEK, Marjan. Ni-YSZ SOFC anodes : minimization of carbon deposition. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, no. 2/3, str. 487-491, graf. prikazi. [COBISS.SI-ID 28414981]

ATM6. DASSENOY, F., JOLY-POTTUZ, L., MARTIN, J. M., VRBANIĆ, Daniel, MRZEL, Aleš, MIHAILOVIĆ, Dragan, VOGEL, W., MONTAGNAC, G. Tribological performances of Mo[sub]6S[sub]3I[sub]6 nanowires. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, no. 2/3, str. 915-919, ilustr. [COBISS.SI-ID 28476421]

ATM7. MARINŠEK, Marjan, PEJOVNIK, Stane, MAČEK, Jadran. Modelling of electrical properties of Ni-YSZ composites. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, no. 2/3, str. 959-964, graf. prikazi. [COBISS.SI-ID 28415237]

ATM8. VRBANIĆ, Daniel, PEJOVNIK, Stane, MIHAILOVIĆ, Dragan, KUTNJAK, Zdravko. Electrical conductivity of Mo[sub]6S[sub]3I[sub]6 and Mo[sub]6S[sub](4.5)I[sub](4.5) nanowires. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, no. 2/3, str. 975-977, Graf. prikazi. [COBISS.SI-ID 28263429]

ATM9. RAZPOTNIK, Tanja, MAČEK, Jadran. Synthesis of nickel oxide/zirconia powders via a modified Pechini method. *J. Eur. Ceram. Soc.*. [Print ed.], 2007, vol. 27, no. 2/3, str. 1405-1410, Graf. prikazi. [COBISS.SI-ID 28239109]

ATM10. MARINŠEK, Marjan, ZUPAN, Klementina, RAZPOTNIK, Tanja, MAČEK, Jadran. A co-precipitation procedure for the synthesis of LSM material = Soobarjanje LSM za pripravo katodnih materialov za gorivne celice. *Mater. tehnol.*, mar./apr. 2007, letn. 41, št. 2, str. 85-90. [COBISS.SI-ID 603562]

ATM11. DALLAS, Panagiotis, NIARCHOS, Dimitrios, VRBANIĆ, Daniel, BOUKOS, Nicholaos, PEJOVNIK, Stane, TRAPALIS, Christos, PETRIDIS, Dimitrios. Interfacial polymerization of pyrrole and in situ synthesis of polypyrrole/silver nanocomposites. *Polymer (Guildf.)*. [Print ed.], 2007, vol. 48, no. 7, str. 2007-2013, ilustr. [COBISS.SI-ID 28476933]

ATM12. KIS, András, CSANYI, G., VRBANIĆ, Daniel, MRZEL, Aleš, MIHAILOVIĆ, Dragan, KULIK, A. J., FORRÓ, László. Nanomechanical investigation of Mo[sub]6S[sub](9-x)I[sub]x nanowire bundles. *Small (Weinh., Print)*, 2007, vol. 3, no. 9, str. 1544-1548. [COBISS.SI-ID 20953895]

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

ATM13. DOMINKO, Robert, PEJOVNIK, Stane. Electrochemical wiring in battery materials : [invited lecture]. V: *International Battery Materials Association 2007 conference : Shenzhen, China, November 16-20, 2007*. [S.l.]: International Battery Materials Association, 2007, str. 8-9. [COBISS.SI-ID 3831578]

ATM14. MAČEK, Jadran. Ceramic membrane technologies and processing. V: BioCellus Summer School, 04.09.2007 - 08.09.2007, Seggau Castle, Austria. *Solid oxide fuel cells combined with biomass gasification*. [S. l.: s. n.], 2007, str. 1-35. [COBISS.SI-ID 29222661]

ATM15. MARINŠEK, Marjan. Fuel cell materials. V: BioCellus Summer School, 04.09.2007 - 08.09.2007, Seggau Castle, Austria. *Solid oxide fuel cells combined with biomass gasification*. [S. l.: s. n.], 2007, str. 1-24. [COBISS.SI-ID 29222405]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

ATM16. PAPON, Pierre, PEJOVNIK, Stane. S&T policy guidelines for Bosnia and Herzegovina. V: *Why invest in science in South Eastern Europe? : Proceedings of the International conference and High level round table 28-29 sept. 2006, Ljubljana, Slovenija*, (Science policy series, Vol. No.5). Venice: UNESCO-BRESCE, 2007, str. 96-98. [COBISS.SI-ID 29074949]

ATM17. ZUPANČIČ-VALANT, Andreja, ŽUMER, Miha, MARINŠEK, Marjan. Rheological properties of serum separation sealant composed of silica particles in dimethyl polysiloxane : [oral presentation]. V: 4th An-

nual European Rheologu Conference, Napoli, Italy, April 12-14, 2007. *AERC 2007 : book of abstracts*. [S.l.]: European Society of Rheology, 2007, str. 53. [COBISS.SI-ID 28868613]

ATM18. MAČEK, Jadran, NOVOSEL, Barbara, MARINŠEK, Marjan, ZUPAN, Klementina. Carbon deposition on SOFC anodes from biogas : [visual presentation]. V: *From research to market deployment : programme*. Munich: ETA: WIP, 2007, str. 94. [COBISS.SI-ID 29226757]

ATM19. MARINŠEK, Marjan, ZUPAN, Klementina, MAČEK, Jadran. Temperature profile analysis during the combustion synthesis of doped lanthanum gallate = Analiza temperaturnih profilov med zgorevalno sintezo dopiranega lantanovega galata. V: JENKO, Monika (ur.). 15. konferenca o materialih in tehnologijah = 15th Conference on Materials and Technology, 8-10 October, 2007 Portorož, Slovenia. *Program in knjiga povzetkov*. Ljubljana: Inštitut za kovinske materiale in tehnologije], 2007, str. 124. [COBISS.SI-ID 29224709]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

ATM20. PEJOVNIK, Stane. Designing of electrode properties in Li ion batteries : [Institute of Chemistry, Universidade Estadual Paulista, on february 6, 2007, Araraquara, SP, Brazil]. Araraquara, 2007. [COBISS.SI-ID 28883461]

UREDNIK / EDITOR

ATM21. *Acta chimica slovenica*. Pejovnik, Stane (Steering Committee Member 1998-). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993-. ISSN 1318-0207. http://acta.chemsoc.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
prof. dr. Valentin Koloini (do / *till* 30. 09. 2007)
akademik prof. dr. Janez Levec
prof. dr. Miha Žumer (do / *till* 30. 09. 2007)
prof. dr. Aleksander Pavko
prof. dr. Marin Berovič
izr. prof. dr. Igor Plazl
izr. prof. dr. Jana Zagorc Končan

Asistenti / Assistants
doc. dr. Ana Lakota Družina
doc. dr. Andreja Zupančič Valant
doc. dr. Andreja Žgajnar Gotvajn
doc. dr. Polona Žnidaršič Plazl
David Senica, univ. dipl. ing. (do / *till* 31. 08. 2007)

Tehniki / Technicians
Klemen Birtič (od / *since* 15. 12. 2007)
Vesna Delalut
Dušan Komel

Mladi raziskovalci Young Researchers	Mentor Mentor	Čas usposabljanja Programme Duration	Oblika usposabljanja Degree
Andrej Pohar	I.Plazl	2007–2012	doktorski študij / *PhD*
Janja Babič	A. Pavko	2005–2010	doktorski študij / *PhD*
Mirjan Švagelj	M. Berovič (študijski mentor B. Štrukelj)	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

Dodiplomski programi / *Undergraduate Programmes*

Prenos toplote in snovi / *Heat and Mass Transfer* – UNI

Osnove kemijske tehnike / *Fundamentals of Chemical Engineering* – VSŠ

Načrtovanje procesov in ekološko inženirstvo / *Process Design and Ecological Engineering* – UNI

Kemijsko reakcijsko inženirstvo / *Chemical Reaction Engineering* – UNI

Osnove kemijske tehnike / *Fundamentals of Chemical Engineering* – UNI

Biotehnologija / *Biotechnology* – UNI

Pregled biokemijskih tehnologij / *Biotechnological Processes* – UNI

Biokemijsko inženirstvo in biotehnologija / *Biochemical Engineering and Biotechnology* – UNI

Biotehnologija z biokemijskim inženirstvom / *Biotechnology and Biochemical Engineering* – UNI

Mehanske operacije / *Mechanical Operations* – VSŠ

Kemijska inženirska kinetika / *Chemical Engineering Kinetics* – VSŠ

Načrtovanje procesov in naprav / *Process and Equipment Design* – VSŠ

Kemija okolja / *Environmental Chemistry* – UNI

Ekološko inženirstvo / *Ecological Engineering* – UNI

Varstvo okolja / *Environmental Engineering* – VSŠ

Industrijska ekologija in ekološko inženirstvo / *Industrial Ecology and Engineering* – VSŠ

Kemijsko procesno računstvo / *Chemical Process Calculations* – UNI

Modeliranje procesov / *Process Modeling* – UNI

Načrtovanje procesov in naprav / *Process and Equipement Design*– VSŠ

Industrijska ekologija in ekološko inženirstvo / *Industrial Ecology and Engineering* – VSŠ

Kemijsko inženirski praktikum / *Chemical Engineering Practice* – UNI

Kemijsko inženirski praktikum / *Chemical Engineering Practice* – VSŠ

Podiplomski programi / *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

Dodiplomski programi / *Undergraduate Programmes*

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

Bioprocesništvo / *Bioprocess Engineering* BF – UNI

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

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

Podiplomski programi / *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*

b. Raziskave s področja biokemijskega inženirstva / *Research in the Field of Biochemical Engineering*

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

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE IN PRIZNANJA / AWARDS, RECOGNITIONS

– Jerica Strniša, Krkina nagrada za diplomsko delo v letu 2007 / *The Krka Award for BSc Thesis in 2007*

ODMEVNI ZNANSTVENI DOSEŽKI / SCIENTIFIC ACHIEVEMENTS

– M. Berovič, patentna aplikacija, 3 znanstveni članki, 2 poglavji v monografiji, sekcija na Evropskem kongresu biotehnologije, plenarno predavanje */ Patent Application, Three Scientific Publications, Two Chapters in a Monograph, Plenary Lecture at the European Congress on Biotechnology*

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

– V. Koloini, *Chemical and Biochemical Engineering Quarterly (*do - *till - 30. 09. 2007)*
– I. Plazl, *Chemical and Biochemical Engineering Quarterly (*od - *since - 01. 10. 2007)*
– A. Pavko, glavni urednik / *Editor-in-Chief, Acta Chimica Slovenica*
– A. Pavko, *Food Technology and Biotechnology*
– M. Berovič, *EFB New Biotechnology – Editor, Biochemical Engineering 2007, Journal of European Federation on Biotechnology, Elsevier, Amsterdam.*
– M. Berovič, *Associate Editor, Biotechnology Annual Review*

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

– M. Berovič, podpredsednik in član znanstvenega in organizacijskega odbora / *Vice President and Member of the Scientific and Organisation Committee, IMMC4 : 4th International Medicinal Mushroom Conference, 23–27 September 2007, Ljubljana, Slovenia.*
– M. Berovič, član znanstvenega programskega odbora */ Member of the Scientific and Programme Committee, 13 th European Congress on Biotechnology, 16–19 September 2007, Barcelona, Spain*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Plinski kromatograf HP / *Gas Chromatograph HP*
- Tekočinski kromatograf Knauer / *HPLC Knauer*
- 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*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P2-0191 Kemijsko inženirstvo/ *Chemical Engineering*
Vodja programa / *Principal Researcher:* V. Koloini (do 30. 09. 2007) / M. Krajnc (od 01. 10. 2007)

P2-0150 Integralni pristop k preprečevanju onesnaževanja voda / *Integrated Approach to Water Pollution Prevention*
Vodja programa / *Principal Researcher:* M. Roš (KI)

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L4-6420 Produkcija farmacevtsko aktivnih spojin *Grifola frondosa* s postopkom gojenja na trdnem in tekočem gojišču / *Production of Pharmaceutically Active Compounds from Grifola Frondosa by Solid State and Submerged Cultivation*
Nosilec / *Principal Researcher:* M. Berovič
Sofinancer / *Co-sponsored by*: ZRS Bistra Ptuj

L4-7595 Razvoj sistema za procesno vodenje fermentacij v vinarstvu / *Development of Process Control System for Wine Fermentation*
Nosilec / *Principal Researcher:* M. Berovič
Sofinancer / *Co-sponsored by*: ZRS Bistra Ptuj

L2-7589 Nadaljna uporaba sekundarnih surovin živilsko predelovalne industrije v Podravju za gojenje jedilnih in farmacevtsko zanimivih gob / *Application of Food Technology Secondary Wastes of Podravje Region for Cultivation of Edible and Medicinal Mushrooms*
Nosilec / *Principal Researcher:* M. Berovič
Sofinancer / *Co-sponsored by*: ZRS Bistra Ptuj

DARS d.d., št. 1163/06 Izvedba študij za projektiranje, ekonomiko, tehnologijo in varovanje okolja: Vpliv zamenjave kamene moke s hidratiziranim apnom v asfaltnih zmeseh za obrabne in zaporne plasti / *Research Projects on Planning, Economics, Technology and Environment Protection*: *Influence of Hydratised Lime on Mechanical Properties of Bitumen Binders*
Nosilec / *Principal Researcher:* A. Zupančič Valant
Financer / *Sponsored by:* DARS d.d.

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

Raziskave na področju membranskih separacijskih tehnik / *Research in the Field of Membrane Separation Techniques*
Nosilec / *Principal Researcher*: A. Pavko
Financer / *Sponsored by:* Lek d.d., Ljubljana.

Anaerobna soobdelava odpadne farmacevtske brozge – micelija s travno-koruzno silažo in svinjsko gnojevko / *Anaerobic Stabilization of Waste Fermentation Broth Using Grass-Corn Silage and Pig Slurry*
Nosilec / *Principal Researcher*: J. Zagorc Končan
Financer / *Sponsored by*: Lek d.d., Lendava

Optimiranje delovanja komunalnih naprav z dodatkom bioaktivnih preparatov / *Optimization of Municipal Systems with Addition of Complex Bioactive Activators.*
Nosilec / *Principal Researcher*: A. Žgajnar Gotvajn
Financer / *Sponsored by*: DARS – Družba za avtoceste Republike Slovenije

1/MK/2007 Razvoj novega materiala za jedro panela iz ekspandiranega perlita – faza IV / *Development of New Material for Panel Core from Expanded Perlite-IV*
Nosilec / *Principal Researcher*: I. Plazl
Financer / *Sponsored by*: Trimo Trebnje d.d., Trebnje

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovanija – Češka *Slovenia – Czech Republic*	Biodegradacija industrijskih organskih barvil z imobiliziranimi ligninolitičnimi glivami / *Biodegradation of Industrial Organic Dyes with Immobilized Ligninolytic Fungi* Nosilec / *Principal Researcher*: A. Pavko
Slovenija – Slovaška *Slovenia – Slovak Republic*	Metodologija vrednotenja izboljšanja sposobnosti biološkega čiščenja močno onesnaženih odpadnih vod s kemijskimi postopki / *Methodology for the Evaluation of Biotreatability Improvement of Heavily Polluted Wastewater after Chemical Treatment* Nosilec / *Principal Researcher:* A. Žgajnar Gotvajn
Slovenija – Kitajska *Slovenia – China*	Produkcija farmacevtsko aktivnih spojin *Grifola frondoza* s postopkom gojenja na trdnem in tekočem gojišču / *Production of Pharmaceutically Active Compounds from Grifola Frondosa by Solid State and Submerged Cultivation* Nosilec / *Principal Researcher:* M. Berovič

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

M. Berovič, prijava in organizacija dveh EC Framework 7 projektov / *Application and Organisation of Two FP 7 Projects:*

Production of Immunotherapeutic Biomolecules from Agricultural Industrial Wastes by Ganoderma Lucidum

Biotechnology for the Conversion of Agricultural Production, Forestry and Biological Industries Wastes into Edible and Medicinal Mushrooms – The Source of Proteins, Vitamins, Mineral Elements and Biologically Active Substances

VABLJENA PREDAVANJA NA INSTITUCIJAH V SLOVENIJI / INVITED LECTURES IN SLOVENIA

- M. Berovič, M. Herga, Vpliv temperaturnega šoka na vcepek Saccharomyces cerevisiae in produkcijo glicerola v vinih / *Influence of Heat Shock on Saccharomyces Cerevisiae Inoculum and Glycerol Biosynthesis*, *Vinarski dan, Ljubljana, June 2007*
- M. Berovič, B. Boh, B. Wraber-Herzog, F. Pohleven, *Production of Intra – and Extracelluar Polysaccharides of Grifola Frondosa, The Fourth International Medicinal Mushroom Conference : IMMC4, September 2007, Ljubljana*

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

- M. Berovič, D. A. Mitchell, *Production of Fungal Enzymes by Solid State Fermentation; Plant & Microbial Enzymes: Isolation, Characterization & Biotechnology Applications,* Tbilisi, Georgia, July 2007
- M. Berovič, *Grifola Frondosa and its Pharmaceutically Active Compounds*, Edible Mushroom Institute, Shanghai, China, June 2007
- M. Berovič, *Design and Operation of Bioreactors for Solid State Bioprocessing; Symbiosis: Science, Industry & Society,* Barcelona, Spain, September 2007
- I. Plazl, *Studies at the Microreactor Scale; Symbiosis: Science, Industry & Society,* Barcelona, Spain, September 2007
- A. Žgajnar Gotvajn, *Challenges for Environmental Engineers in Slovenia,* Slovak University of Technology, Faculty of Chemical and Food Technology, Institute of Chemical and Environmental Engineering, Bratislava, Slovak Republic, September 2007

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

- Prof. Dr. J. Decro, Prof. Dr. M. Drtil, Slovak University of Technology, Faculty of Chemical and Food Technology, Institute of Chemical and Environmental Engineering, *Application of Ozone for Wastewater Treatment,* April 2007

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Blaž Likozar	M. Krajnc	2004–2009	doktorski študij / *PhD*
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Sašo Rogelj	M. Krajnc	2003–2008	doktorski študij / *PhD*
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- Uvod v tehnologijo / *Introduction to Technology* – VSŠ
- Organski procesi in produkti / *Organic Processes and Products* – VSŠ
- Osnove kemijskih tehnoloških procesov / *Fundamentals of Technological Processes* – UNI
- Organska tehnologija I / *Organic Chemical Technology I* – UNI
- Polimeri / *Polymers* – UNI
- Separacijski procesi / *Separation Processes* – UNI
- Organski materiali in produkti / *Organic Materials and Products* – UNI

Podiplomski programi / *Postgraduate Programmes*

- Kemija in tehnologija posebnih polimerov / *Chemistry and Technology of Advanced Polymer Materials*
- Struktura in stereokemija polimerov / *Structure and Stereochemistry of Polymers*
- Izbrana poglavja iz termodifuzijskih operacij / *Selected Topics of Separation Processes*

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Dodiplomski programi / *Undergraduate Programmes*

- Polimerni materiali / *Polymer Materials* BF – UNI
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RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

- Študij kinetike med vulkanizacijo različnih gumenih zmesi / *Kinetic Investigations During Vulcanization Processes of Different Rubber Blends*
- Študij prenosa toplote med vulkanizacijo različnih gumenih zmesi / *Heat Transfer Investigations During Vulcanization Processes of Different Rubber Blends*
- Raziskave vezivnih sistemov za gumarsko industrijo / *Research of Adhesion Bonding Systems in Rubber Industry*
- 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*
- 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*
- Raziskave na področju ekspanzijskega injekcijskega stiskanja / *Research in the Field of Injection Blow Molding*
- Aplikativne, procesno inženirske raziskave proizvodov na osnovi fosfornih spojin prve generacije in produktno inženirske raziskave nove generacije proizvodov / *Applied Process Engineering Research of First Generation Products Based on Phosphoric Substances and Product Engineering Research of New Generation 3E+C Products*
- 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*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

- Mednarodna konferenca / *International Conference: »European Polymer Congress«*, Portorož, July 2007

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
– Pilotni tankoslojni uparjalnik / *Pilot Plant Thin-Film Evaporator*

SODELOVANJE V TEHNOLOŠKIH MREŽAH IN PLATFORMAH / TECHNOLOGY NETWORKS & PLATFORMS

– Tehnološka mreža: Inteligentni polimerni materiali in pripadajoče tehnologije / *Technology Network: Intelligent Polymer Materials and Technologies*
– Tehnološka platforma NaMaT: Napredni materiali in tehnologije / *Technology Platform NaMaT: Advanced Materials and Technologies*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P2-0191 Kemijsko inženirstvo/ *Chemical Engineering*
Vodja programa / *Principal Researcher:* V. Koloini (do 30. 09. 2007) / M. Krajnc (od 01. 10. 2007)

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L2-6344 Aplikativne, procesno inženirske raziskave proizvodov na osnovi fosfornih spojin prve generacije in produktno inženirske raziskave nove 3E+I generacije proizvodov / *Applied Process Engineering Research of First Generation Products Based on Phosphoric Substances and Product Engineering Research of New Generation 3E+C Products*
Nosilec / *Principal Researcher:* J. Golob
Sofinancer / *Co-sponsored by*: TKI Hrastnik

L2-6686 Vezivni sistemi v gumenih kompozitih z izboljšano površinsko aktivnostjo / *Rubber Composites – Adhesion Bonding Systems with Improved Surface Activity*
Nosilec / *Principal Researcher:* M. Krajnc
Sofinancer / *Co-sponsored by*: Goodyear EPE

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

Testiranje gume in gumenih kompozitov / *Rubber and Rubber Composites Testing*

Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Goodyear EPE

Raziskave in razvoj na področju formaldehidnih smol / *Research and Development of Formaldehyde Resins*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Nafta Petrochem

Povečanje konkurenčne sposobnosti izdelkov na osnovi multifunkcionalnih polimernih materialov / *Enhancing Market Competitiveness of Products Based on Multifunctional Polymer Materials*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Goodyear EPE

Melaminske pene / *Melamine Foams*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Melamin Kočevje

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

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IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

POT1. LIKOZAR, Blaž, KRAJNC, Matjaž. Temperature dependent dynamic mechanical properties of hydrogenated nitrile butadiene rubber and the effect of peroxide cross-linkers. *E-polymers*. [Online ed., http://www.e-polymers.org/], 2007, no. 131, str. 1-20. [COBISS.SI-ID 29085957]

POT2. ŠEBENIK, Urška, KRAJNC, Matjaž. Influence of the soft segment lenght and content on the synthesis and properties of isocyanate-terminated urethane prepolymers. *Int. j. adhes. adhes.*. [Print ed.], 2007, vol. 27, no. 7, str. 527-535, ilustr. [COBISS.SI-ID 28640005]

POT3. LIKOZAR, Blaž, KRAJNC, Matjaž. Kinetic and heat transfer modeling of rubber blends' sulfur vulcanization with N-t-butylbenzothiazole-sulfenamide and N,N-di-t-butylbenzothiazole-sulfenamide. *J. appl. polym. sci.*, 2007, vol. 103, no. 1, str. 293-307, Graf. prikazi. [COBISS.SI-ID 28051973]

POT4. POLJANŠEK, Ida, LIKOZAR, Blaž, KRAJNC, Matjaž. Kinetics of hydroxymethyl phenols formation by in-line FTIR spectroscopy. *J. appl. polym. sci.*, 2007, vol. 106, no. 2, str. 878-888. [COBISS.SI-ID 28751877]

POT5. VIDIČ, Jana, PODGORNIK, Aleš, JANČAR, Janez, FRANKOVIČ, Vida, KOŠIR, Boštjan, LENDERO, Nika, ČUČEK, Karmen, KRAJNC, Matjaž, ŠTRANCAR, Aleš. Chemical and chromatographic stability of methacrylate-based monolithic columns. *J. chromatogr.*, 2007, vol. 1144, no. 1/2, str. 63-71, ilustr. [COBISS.SI-ID 28598021

POT6. LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Modeling of dynamic mechanical properties of vulcanized fluoroelastomer. *Polym. eng. sci.*, 2007, vol. 47, no. 12, str. 2085-2094. [COBISS.SI-ID 29035781]

POT7. VRLINIČ, Tjaša, VESEL, Alenka, CVELBAR, Uroš, KRAJNC, Matjaž, MOZETIČ, Miran. Rapid surface functionalization of poly(ethersulphone) foils using a highly reactive oxygen-plasma tretament. *Surf. interface anal.*, 2007, vol. 39, no. 6, str. 476-481. [COBISS.SI-ID 20699943]

POT8. KLOFUTAR, Boštjan, GOLOB, Janvit. Microorganisms in diesel and in biodiesel fuels. *Acta chim. slov.*. [Tiskana izd.], 2007, vol. 54, no. 4, str. 744-748. http://acta.chem-soc.si/54/54-4-744.pdf. [COBISS.SI-ID 29169925]

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POT9. LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Hydrogenated acrylonitrile butadiene elastomer/coagent nanocomposites : [oral contribution]. V: *European polymer congress [also] epf, 2-6 july, 2007, Congress centre Bernardin, Portorož, Slovenia*. Ljubljana: Slovenian Chemical Society, 2007, str. [1-2], ilustr. [COBISS.SI-ID 28754181]

POT10. KAJTNA, Jernej, KRAJNC, Matjaž, GOLOB, Janvit. Microsphere acrylic pressure sensitive adhesives : the influence of process and chemical parameters on adhesion properties : [oral contribution]. V: *European polymer congress [also] epf, 2-6 july, 2007, Congress centre Bernardin, Portorož, Slovenia*. Ljubljana: Slovenian Chemical Society, 2007, str. [1-2]. [COBISS.SI-ID 28754437]

POT11. MOHORKO, Jošt, POLJANŠEK, Ida, KRAJNC, Matjaž. Synthesis and characterization of melamine-formaldehyde prepolymer for the manufacture of the resilient foams. V: *European polymer congress [also] epf, 2-6 july, 2007, Congress centre Bernardin, Portorož, Slovenia*. Ljubljana: Slovenian Chemical Society, 2007, str. [1-2], ilustr. [COBISS.SI-ID 28755205]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

POT12. KRAJNC, Matjaž, ŠEBENIK, Urška. *Poročilo : o delu po pogodbi št. R001/2007 za MELAMIN kemična tovarna d.d. Kočevje*. Ljubljana: Univerza V Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo, 2007. 37 f., ilustr. [COBISS.SI-ID 29183493]

POT13. KRAJNC, Matjaž, ŠEBENIK, Urška. *Razvoj testne metode abrazije zobatega pogonskega jermena : Razvojno investicijski projekt: povečanje konkurenčne sposobnosti izdelkov na osnovi multifunkcionalnih polimernih materialov : Prvo fazno poročilo raziskave : za Goodyear Engineered Products Europe, d.o.o. : Ljubljana, 05/01/2007*. Ljubljana: Univerza v Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo, 2007. 24 f., ilustr. [COBISS.SI-ID 28322053]

POT14. POLJANŠEK, Ida, KRAJNC, Matjaž. *Vpliv procesnih parametrov na sintezo prepolimera za izdelavo melaminsko-formaldehidne pene : Letno poročilo o delu po pogodbi št. R001/2006 med Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani in Melaminom d.d., Kočevje, Kemična tovarna*. Ljubljana: Univerza V Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo, 2007. [52] f., graf. prikazi. [COBISS.SI-ID 28413957]

UREDNIK / EDITOR

POT15. GOLOB, Janvit (ur.), FALETIČ, Mateja (ur.). *Zbornik referatov s posveta Prodaja državnega premoženja, Ljubljana, 12. aprila 2007*. Ljubljana: Državni svet Republike Slovenije, 2007. ISBN 978-961-6453-19-6. [COBISS.SI-ID 236150784]

KATEDRA ZA VARSTVO PRI DELU
CHAIR OF SAFETY AT WORK

PREDSTOJNIK KATEDRE / HEAD

mag. Jože Šrekl, viš. pred.

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
dr. Mitja Robert Kožuh, viš. pred.
mag. Jože Šrekl, viš. pred.
mag. Aleš Jug, pred.
prof. dr. Stojan Petelin

Asistenti / Assistants
Marjan Lukežič, univ. dipl. ing.

Tehniki / Technicians
Iztok Košir
Miran Banfi

Administrativno osebje / Administration
Slavka Lobnik

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski program / *Professional Study Programme*

Matematika I / *Mathematics* – VSŠ

Tehniška mehanika / *Technical Mechanics* – VSŠ

Računalništvo / *Computer Science* – VSŠ

Osnove varstva pri delu / *Basics of Safety at Work* – VSŠ

Izbrana poglavja iz matematike in statistike / *Selected Topics in Mathematics and Statistics* – VSŠ

Varstvo okolja I / *Environmental Protection I* – VSŠ

Teorija gorenja, gašenja in dinamika požarov / *Theory of Combustion, Extinction and Fire Dynamics* – VSŠ

Delovno okolje – Prezračevanje / *Working Environment – Ventilation* – VSŠ

Delovno okolje – Hrup / *Working Environment – Noise* – VSŠ

Psihologija dela / *Occupational Psychology* – VSŠ

Varstvo okolja II / *Environmental Protection II* – VSŠ

Medicina in higiena dela / *Medicine and Occupational Hygiene* – VSŠ

Ergonomija in ergonomske meritve / *Ergonomy and Ergonomic Measurements* – VSŠ

Varnost delovnih priprav in naprav / *Safety of Machinery and Equipment* – VSŠ

Gašenje požarov in reševanje / *Fire Fighting and Rescue* – VSŠ

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 Equations 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

– Mojca Malovrh, Nagrada Avgusta Kuharja za najboljše diplomsko delo za leto 2007 / *The Avgust Kuhar Award for the Best Diploma Work for 2007*

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL MEETINGS

– Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož, maj 2007, / *Safety at Work, Fire Safety and Occupational Medicine, Two Days Symposium with International Participation, Portorož, May 2007*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L2-6471	Razvoj metodologij za oceno tveganj v cestnih predorih / *Development of Methodologies for Risk Analysis of Road Tunnels* Nosilec / *Principal Researcher:* S. Petelin (UL FPP) Sofinancer / *Co-sponsored by*: DARS – Družba za avtoceste v RS
M5-0147	Razvoj učnih sredstev za ugotavljanje varstva pred požarom / *Development of Learning Means Used for Fire Protection* Nosilec / *Principal Researcher*: P. Bukovec Sofinancer / *Co-sponsored by*: Ministrstvo za obrambo RS

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI V RS / COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS IN SLOVENIA

PHARE projekt: Čili za delo; sodelovanje s Kliničnim inštitutom medicine dela, prometa in športa / *Project PHARE: Fit for Work; Collaboration with the Clinical Institute of Occupational, Traffic and Sports Medicine*

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IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

OTV1. AL-MANSOUR, Fouad, KOŽUH, Mitja. Risk analysis for CHP decision making within the conditions of an open electricity market. *Energy (Oxford)*. [Print ed.], 2007, vol. 32, no. 10, str. 1905-1916. [COBISS.SI-ID 20987431]

OTV2. KOŽUH, Mitja, PETELIN, Stojan, PERKOVIČ, Marko. Can classification societies with their rules on redundancy propulsion improve statistics on oil spills and cleaning costs?. *Mar. eng. (Tokyo)*, 2007, vol. 42, no. 3, str. 113-118, graf. prikazi. [COBISS.SI-ID 28861445]

OTV3. VIDMAR, Peter, PETELIN, Stojan. Application of CFD method for risk assessment in road tunnels. *Engineering applications of computational fluid mechanics*, 2007, vol.1, no. 4, str. 273-287. [COBISS.SI-ID 1813091]

OTV4. VIDMAR, Peter, PETELIN, Stojan. Methodology of using CDF-based risk assessment in road tunnels. *Therm.sci.*, 2007, vol. 11, no. 2, str. 223-250. [COBISS.SI-ID 1788259]

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

OTV5. JUG, Aleš, PETELIN, Stojan, BUKOVEC, Peter. Fire behavior in underground car park buildings. V: MAHER, Tomaž (ur.), HERNAVS, Boštjan (ur.). *Transport research : proceedings*, (TransSlo). Ljubljana: Electrotechnical Association of Slovenia, 2007, 2007, 6 f. [COBISS.SI-ID 1746787]

OTV6. VIDMAR, Peter, PETELIN, Stojan. CDF - based methodology for risk assesment in road tunnels. V: MAHER, Tomaž (ur.), HERNAVS, Boštjan (ur.). *Transport research : proceedings*, (TransSlo). Ljubljana: Electrotechnical Association of Slovenia, 2007, 15 f. [COBISS.SI-ID 1746275]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

OTV7. MOLAN, Marija, MOLAN, Gregor, PETELIN, Stojan, KOŽUH, Mitja. Identification of qualitative and qunatitative elements of human behaviour and their inclusion in risk assesment models. V: MAHER, Tomaž (ur.), HERNAVS, Boštjan (ur.). *Applications of intelligent transport systems : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2007, 4 f., ilustr. [COBISS.SI-ID 28775941]

OTV8. PETELIN, Stojan, KOŽUH, Mitja, PERKOVIČ, Marko, VIDMAR, Peter, DAVID, Matej. North Adriatic tanker traffic safety and LNG terminal operation. V: MAHER, Tomaž (ur.), HERNAVS, Boštjan (ur.). *Applications of intelligent transport systems : proceedings*. Ljubljana: Electrotechnical Association of Slovenia, 2007, 2007, 8 f. [COBISS.SI-ID 1747043]

OTV9. KOŽUH, Mitja, PETELIN, Stojan, VIDMAR, Peter, KOŠIR, Iztok. Ocena vplivov na okolje zaradi plinskih terminalov. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2007, 15.-16. 5. 2007*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2007, str. [1-9]. [COBISS.SI-ID 29186053]

OTV10. LUKEŽIČ, Marjan. Predstavitev postopka računalniškega modeliranja razvoja požara v tovornem delu potniškega letala. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2007, 15.-16. 5. 2007*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2007, str. 1-26. [COBISS.SI-ID 29187589]

OTV11. ŠREKL, Jože. Problematika VPD pri starajoči se generaciji. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2007, 15.-16. 5. 2007*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2007, str. [1-9]. [COBISS.SI-ID 29186565]

OTV12. JUG, Aleš. Optimization of parcel logistics. V: MAHER, Tomaž (ur.), HERNAVS, Boštjan (ur.). *Transport research : proceedings*, (TransSlo). Ljubljana: Electrotechnical Association of Slovenia, 2007, [4] f. [COBISS.SI-ID 17431782]

OTV13. JUG, Aleš, PETELIN, Stojan, BUKOVEC, Peter. Fire behavior in underground car park buildings. V: MAHER, Tomaž (ur.), HERNAVS, Boštjan (ur.). *Transport research : proceedings*, (TransSlo). Ljubljana: Electrotechnical Association of Slovenia, 2007, f. [1-6], ilustr. [COBISS.SI-ID 28596485]

OTV14. JUG, Aleš. Ocena požarne nevarnosti kot element koncepta požarne varnosti. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2007, 15.-16. 5. 2007*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2007, str. [1-11]. [COBISS.SI-ID 29187333]

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

OTV15. BEŠTER-ROGAČ, Marija, GSPAN, Primož, JUG, Aleš, KOŠIR, Iztok, PUC, Miha Dominik, TOMŠIČ, Matija. *Praktikum*. Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2007. 130 str., ilustr. ISBN 978-961-6286-76-3. [COBISS.SI-ID 229928192]

DRUGO UČNO GRADIVO / OTHER EDUCATIONAL MATERIAL

OTV16. LUKEŽIČ, Marjan, JUG, Aleš. *Navodila za pisanje strokovnega poročila o delovni praksi študentov Oddelka za tehniško varnost : interno gradivo, marec 2007*. Ljubljana: Univerza v Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, 2007. 8 f. [COBISS.SI-ID 28516357]

KONČNO POROČILO O REZULTATIH RAZISKAV / FINAL RESEARCH REPORT

OTV17. PETELIN, Stojan, VIDMAR, Peter, PERKOVIČ, Marko, KOŽUH, Mitja, PALISKA, Dejan, MOLAN, Marija, MODIC, Jurij, VALIČ, Marko, STIJEPIĆ, Andrej, LUIN, Blaž. *Razvoj metodologij za oceno tveganj v cestnih predorih = Aplikativni raziskovalni projekt : zaključno poročilo za obdobje 2004-2007*. Portorož: Univ., Ljubljana, Fak. za pomorstvo in promet, 2007. 65 str., ilustr. [COBISS.SI-ID 1798755]

DRUGA IZVEDENA DELA / OTHER PERFORMED WORKS

OTV18. JUG, Aleš. *Nastanek in razvoj požara ter evakuacija iz objekta : [Univerza v Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo, Ljubljana, dne 22.1.2007]*. Ljubljana, 2007. [COBISS.SI-ID 28308997]