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

POROČILO O IZOBRAŽEVALNI IN RAZISKOVALNI DEJAVNOSTI V LETU 2008

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ANNUAL REPORT 2008

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KAZALO

UVODNA BESEDA

Veseli me, da prebirate Poročilo o izobraževalni in raziskovalni dejavnosti v letu 2008, ki smo ga pripravili na Fakulteti za kemijo in kemijsko tehnologijo, Univerze v Ljubljani (FKKT UL). Preteklo leto je bilo za fakulteto in njene sodelavce v marsičem prav posebno leto.

Ponosni smo predvsem na naslednje dosežke:

1. Pripravili smo vse študijske programe, ki so skladni z bolonjsko reformo in dobili zanje akreditacijo pri Svetu za visoko šolstvo. Vsi programi so bili sprejeti z najširšim soglasjem učiteljev in so dobili izjemno visoke ocene strokovnih recenzentov. V šolskem letu 2009/2010 bomo prvič vpisovali v prenovljene programe prve stopnje in v nov doktorski študijski program Kemijske znanosti, ki ima tri usmeritve: kemija, biokemija in kemijsko inženirstvo. Predstavitvene zbornike vseh programov si lahko ogledate na naših domačih straneh. Odločili smo se, da bomo programe akreditirali tudi mednarodno (ECTN in FEANI).
2. Poročila o delu programskih skupin so daljša kot pretekla leta, ker zajemajo celotno obdobje financiranja (2004–2008). Letošnje poročilo zato podaja celovito sliko o znanstvenih in drugih pomembnih dosežkih sodelavcev fakultete v zadnjih petih letih. V letu 2008 se je izteklo že drugo obdobje »programskega financiranja« in z zadovoljstvom sporočamo, da smo bili na razpisu za novo, tretje obdobje izjemno uspešni. To dokazuje, da smo raziskovalna visokošolska ustanova.
3. Dokončali smo zahtevno pripravo dokumentacije, potrebne za pridobitev gradbenega dovoljenja za novo stavbo na lokaciji Brdo. Sodelovanje s službo za investicije Univerze v Ljubljani, s projektanti, predvsem pa s kolegi s Fakultete za računalništvo in informatiko je bilo zgledno in uspešno. Pripravili smo tudi investicijsko dokumentacijo za finančno pomoč Evropskega sklada za regionalni razvoj/Kohezijski sklad.

S ponosom lahko zatrdim, da smo v letu 2008 uspešno delali in dosegli lepe rezultate ter potrdili visoko kvaliteto delovanja. Trdno sem prepričan, da bomo v akademski skupnosti profesorjev, raziskovalcev in študentov izpolnili tudi smele načrte, ki jih imamo za prihodnost.

Kot dekan pa bi se rad zahvalil vsem sodelavcem Fakultete za kemijo in kemijsko tehnologijo za uspešno delo.

Dekan:
prof. dr. Stane Pejovnik

FOREWORD

We are glad to present you the Report on Educational and Research Activities of the Faculty of Chemistry and Chemical Technology, University of Ljubljana for 2008. Last year was a special year for us in many ways and we are particularly proud of the following achievements:

We have managed to prepare and adapt all our study programmes according to the Bologna reform and have received accreditation from the Council for Higher Education. We are glad that all the programmes have been accepted with a broad consensus of teachers and received high assessment grades from professional reviewers. This means that in the following academic year 2009/2010 students will be enrolled to the new first-cycle study programmes and a new doctoral programme in Chemical Sciences with three options: Chemistry, Biochemistry and Chemical Engineering. You can find information about our programmes on our web site. We have also decided to accredit programmes internationally (ECTN and FEANI).

1. *The reports from our research programme groups are more extensive than in previous years and cover the financing period 2004–2008. With this we are giving a complete picture on our scientific and other achievements for the last five years. In 2008, the second programme funding cycle expired and we are pleased to report that our application for funding in the third cycle has been extremely successful so far which proves that we are truly a research oriented university institution.*
2. *We have also managed to complete documentation for obtaining the building permit for our new premises on the Brdo location. With this we want to acknowledge the help of the Investment service of the University of Ljubljana, design engineers, as well as the colleagues from the Faculty of Computer and Information Science. We have also prepared investment documentation to apply for funding at the European Regional Development Fund.*

We are proud to have achieved so many excellent results and thus confirmed high quality standards of our work. I firmly believe that within the academic community of teachers, researchers and students we are going to fulfil our ambitious plans in the future as well.

As a dean, I would like to express my sincere gratitude to all the associates of the Faculty of Chemistry and Chemical Technology for the excellent work they are performing.

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 Brez kemijskega inženirstva ne bi bilo racionalne proizvodnje neštetih izdelkov, za katere se nam zdi samoumevno, da nam pripadajo.

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

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

POSLANSTVO FAKULTETE

Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani:

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

MISSION STATEMENT

The FKKT members individually and collectively strive to:

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

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST

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

IZOBRAŽEVALNA DEJAVNOST

V letu 2008 se je na FKKT izvajalo pet dodiplomskih študijskih programov:

- univerzitetni program Kemija s smerema
    - Kemija
    - Kemijsko izobraževanje
- univerzitetni program Biokemija
- univerzitetni program Kemijsko inženirstvo
- visokošolski strokovni program Kemijska tehnologija s smermi
    - Kemijska tehnologija
    - Uporabna kemija
- visokošolski strokovni program Varstvo pri delu in požarno varstvo

FKKT je izvajala tudi tri podiplomske študijske programe:

- Kemija
- Kemijsko inženirstvo
- Kemijska tehnologija

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

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

V letu 2008 smo prenovili vse programe v skladu s smernicami bolonjske prenove in vsi so že akreditirani pri Svetu Republike Slovenije za visoko šolstvo. Tako bomo v študijskem letu 2009/10 prvič vpisali študente na prenovljene univerzitetne prvostopenjske programe Kemija, Biokemija, Kemijsko inženirstvo in Tehniška varnost, na prvostopenjski visokošolski strokovni program Kemijska tehnologija ter na prenovljeni doktorski program Kemijske znanosti. Drugostopenjski programi Kemija, Biokemija, Kemijsko inženirstvo, Tehniška varnost in Kemijsko izobraževanje so tudi že dobili akreditacijo Sveta Republike Slovenije za visoko šolstvo, vendar jih v naslednjem študijskem letu še ne bomo izvajali.

Za izvedbo študijskih programov skrbi 32 rednih profesorjev, 17 izrednih profesorjev, 6 docentov, 2 višja predavatelja, 1 predavatelj, 60 asistentov, 3 strokovni sodelavci ter 26 strokovnih delavcev.

RAZISKOVALNA DEJAVNOST

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

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

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

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

VKLJUČENOST V OKOLJE

DODATNO IZOBRAŽEVANJE SREDNJEŠOLCEV IN KEMIJSKA OLIMPIJADA

Na Fakulteti za kemijo in kemijsko tehnologijo smo tudi v letu 2008 organizirali dodatno izobraževanje za srednješolce, ki so nadarjeni za kemijo. V sodelovanju z Zvezo organizacij za tehniško kulturo in Zavodom RS za šolstvo smo dijake povabili na strokovna srečanja, kjer so se srečali s teoretično kemijo, in razvijali svoje spretnosti v laboratoriju. Srednješolci se pri tem seznanijo z najnovejšimi dognanji na področju kemije. Na voljo jim je tudi modelna spletna učilnica, kjer so predstavljene razne kemijske vsebine, ki so na različnih nivojih zahtevnosti.

Jeseni pa smo se na neformalni prireditvi tudi srečali 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 bil dekan FKKT.

Strokovna srečanja potekajo pod vodstvom učiteljev in drugih sodelavcev naše fakultete. Znanje srednješolcev tudi sproti ocenjujemo in testiramo. Med najboljšimi izberemo tudi ekipo, ki se vsako leto udeleži Mednarodne kemijske olimpijade (IChO).

Izbrana slovenska dijaška ekipa je tako v letu 2008 sodelovala na jubilejni 40. mednarodni kemijski olimpijadi v Budimpešti, Madžarska. Več informacij o letošnji olimpijadi lahko najdete s pomočjo spletne povezave: http://www.icho.hu/pages/Home.aspx.

Olimpijada je potekala od 12. 7. do 21. 7. 2008, gostila pa nas je tamkajšnja univerza Eötvös Loránd.

Na tej olimpijadi je sodelovalo 67 držav. Za vsako od njih lahko tekmujejo največ štirje dijaki; v Budimpešti je tekmovalo 259 dijakov.

Slovenske vrste je zastopala naslednja ekipa: Tomaž Mohorič (Gimnazija Bežigrad), Gašper Gregorič in Nemanja Aničić (II. Gimnazija Maribor), ter Nika Anžiček (Gimnazija Brežice). Glavni mentor ekipe na olimpijadi je bil dr. Andrej Godec s Fakultete za kemijo in kemijsko tehnologijo v Ljubljani, drugi mentor pa je bila mag. Breda Novak.

Naša ekipa je na tej olimpijadi dosegla odličen uspeh: eno srebrno medaljo (Tomaž Mohorič) in dve bronasti medalji (Gašper Gregorič in Nemanja Aničić). Ta rezultat je primerljiv z re-

zultati zahodnih držav; na olimpijadah pa so običajno najuspešnejše države daljnega vzhoda (Kitajska, Tajvan, Singapur), Rusija, Iran in tako naprej.

Kemijska olimpijada je sicer tekmovanje gimnazijskih dijakov iz celega sveta v znanju kemije, ki poteka vsako leto. 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 olimpijade. Za dijake je olimpijada izvrstna priložnost, da se srečajo z najbolj nadarjenimi vrstniki iz celega sveta in navežejo dolgoročne stike.

Za vse te dejavnosti aktivno iščemo tudi sponzorje ali donatorje. V letu 2008 je že drugič zapored največ razumevanja za naš projekt v Sloveniji pokazalo podjetje BASF d.o.o.; direktor podjetja gospod Werner Besch in gospa Klementina Homšak sta bila tudi gosta na naši fakulteti. Podjetje BASF d.o.o. je tako postalo glavni donator slovenske dijaške ekipe v letu 2008.

POLETNA ŠOLA KEMIJE 2008

Poletna šola kemije je bila v letu 2008 na naši fakulteti organizirana prvič. Poletne šole se je udeležilo 17 dijakov iz cele Slovenije, potekala pa je prvi teden julija. Udeleženci poletne šole kemije so se s pomočjo predavanj in praktičnih vaj seznanili z različnimi vsebinami in s praktičnimi metodami, ki se uporabljajo v kemiji.

Vodja poletne šole je bil dr. Andrej Godec s Fakultete za kemijo in kemijsko tehnologijo v Ljubljani.

Dijaki so en dan preživeli v laboratoriju Katedre za organsko kemijo, kjer so eksperimentirali pod vodstvom prof. dr. Darka Dolenca in Zdenke Kadunc. Drugi dan so delali v analiznem laboratoriju pod vodstvom prof. dr. Nataše Gros in Jolande Furlan. Tretji dan pa so delali v laboratorijih na Katedri za anorgansko kemijo pod vodstvom doc. dr. Romane Cerc – Korošec in Damjana Erčulja. Zabavno plat kemije sta jim predstavila prof. dr. Ivan Leban in Aleš Knez. Slišali pa so tudi predavanji o sevanju okrog nas (dr. Andrej Godec) in o toksikologiji v povezavi s kemijsko varnostjo (mag. Andreja Bačnik).

Soorganizatorja poletne šole sta bila Zavod RS za šolstvo in Zveza za tehniško kulturo.

Prvi dan v laboratoriju so dijaki delali z rastlinskimi barvili, kot so karotenoidi in klorofili. Ti navadno nastopajo v zmeseh, ki jih lahko uspešno ločujemo s tankoplastno kromatografijo. Dijaki so pri tem poskusu spoznali eno od tehnik kromatografije, ki je danes najbolj razširjena analitska metoda. Poleg tega so izvedli enostavno organsko sintezo aspirina ali paracetamola. Pri tem so dijaki spoznali osnovne prijeme pri delu v sinteznem laboratoriju in osnovne metode karakterizacije organskih spojin.

Drugi dan so se dijaki seznanili z značilnostmi naravnih vod in razlikami v njihovi kemijski sestavi. Spoznali so osnove za vrednotenje kemijske sestave in kakovosti vod. Nadalje so dijaki spoznali nekatere prilagojene laboratorijske postopke za hitro semikvantitativno analizo vzorcev vod. Opravili so laboratorijske analize vzorcev vod, ki so jih sami prinesli. Dobljene rezultate so primerjalno ovrednotili in poskusili čim celoviteje razložiti v povezavi s poznavanjem naravnega okolja, iz katerega so vzorce odvzeli.

Tretji dan v laboratoriju je vsak dijak sam pripravil $FeSO_4 \cdot 7H_2O$ iz elementarnega železa in 20 % raztopine H_2SO_4 in izračunal izkoristek te kemijske reakcije. Osnovni pojmi, s katerimi so se pri tem seznanili, so bili: kemijska enačba, stehiometrično razmerje, prebitek pri kemijski reakciji in izkoristek kemijske reakcije. Pri eksperimentalnem delu so spoznali osnovne postopke preparativne kemije kot so tehtanje, filtriranje ter nučiranje.

Poleg tega so študirali dve ravnotežni reakciji v raztopini na osnovi barv raztopin, ki so posledica prisotnosti določenega koordinacijskega iona. Proučili so vpliv spremembe koncentracije in temperature na ravnotežje. Odgovor na vprašanje, kaj se je zgodilo, so povedale barve.

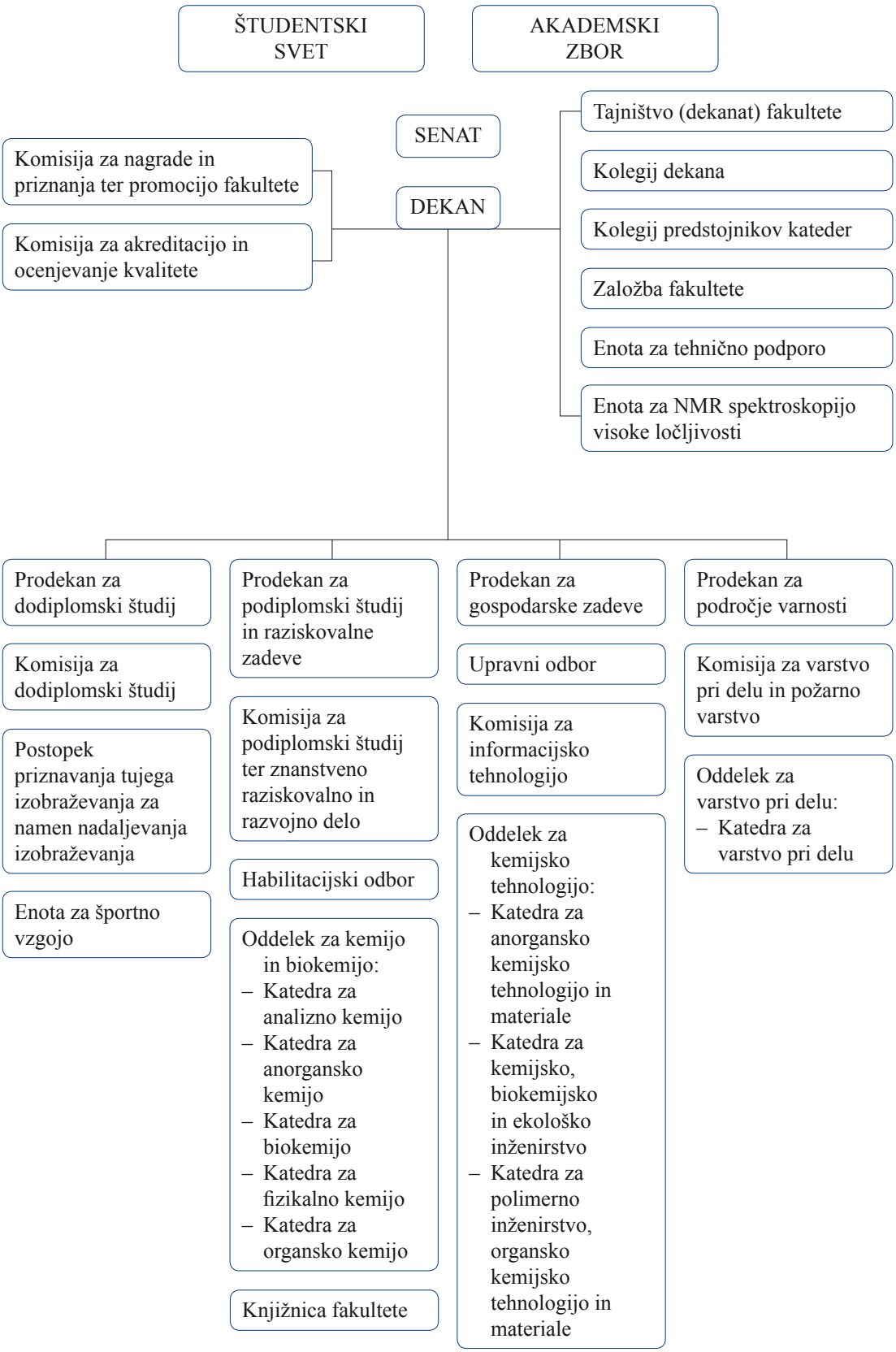
NOČ ZNANSTVENIC IN ZNANSTVENIKOV 2008

Direktorat za znanost in raziskave Evropske komisije je bil tudi v letošnjem letu pobudnik vse-evropskega dogodka z imenom »Noč znanstvenic in znanstvenikov 2008«. Predhodno so bili podobni dogodki že v letih 2005, 2006 in 2007. Bistven namen teh dogodkov je predvsem ta, da bi širšo laično javnost na lahkoten in poučen način seznanili z znanstvenimi dosežki. Hkrati naj bi pri mladih ljudeh vzpodbudili zanimanje za znanost in tehniko. Seveda naj bi sam dogodek popestrili tudi s kemijskimi poskusi.

Dogodki naj bi bili take vrste, da bi bili zanimivi prav za vse – od otrok do starejših. In še več, dogodki naj bi bili predvsem neformalni, prijetni 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 v letih 2006 in 2007 smo tudi v letu 2008, v lastni režiji organizirali »Noč znanstvenic in znanstvenikov 2008«. Nekateri so to prireditev že poimenovali »Noč čarovnic«. Pri organizaciji in izvedbi je sodelovala matična fakulteta, finančni del pa je pokrila programska skupina P1-0175LE. Na prireditvi je bilo skupaj preko 130 obiskovalcev. Izvedli smo vrsto kemijskih poskusov, pri čemer smo uporabili tudi kemikalije, ki jih imamo v gospodinjstvu. Odziv obiskovalcev, tako otrok kot starejših, je bil izreden. Je že tako, da so poskusi v živo povsem drugačni kot oni, ki jih lahko najdete na virtualnem računalniškem spletu. Tako prirediteljem kot obiskovalcem je zato večer ostal v prijetnem spominu.

ORGANIZACIJSKA SHEMA



DIPLOME, MAGISTERIJI IN DOKTORATI V LETU 2008

DIPLOME

UNIVERZITETNI ŠTUDIJSKI PROGRAM

KEMIJA

Jure Bezenšek
Mentor: akademik prof. dr. Branko Stanovnik
Sinteza 8-hidroksiimidazo[1,2-a]piridin-2-karboksilne kisline in njenih derivatov
Datum zagovora: 3. 9. 2008

Rok Borštnar
Mentor: prof. dr. Jurij Lah
Termodinamika vezanja netropsina in distamicina-A na lasnico DNA z veznim mestom AAAAA
Datum zagovora: 24. 4. 2008

Anita Breščak
Mentor: doc. dr. Bogdan Štefane
Sinteza in katalitsko hidrogeniranje alkil in aril substituiranih 2,2-difluoro-1,3,2-dioksaborininov
Datum zagovora: 27. 2. 2008

Matej Černilec
Mentorica: doc. dr. Amalija Golobič
Priprava in strukturna karakterizacija poroznih cinkovih karboksilatov
Datum zagovora: 19. 12. 2008

Nejc Hodnik
Mentor: prof. dr. Boris Pihlar
Ugotavljanje elektrokatalitske aktivnosti Pt katalizatorjev z mikroelektrodo
Datum zagovora: 18. 9. 2008

Amadej Juranovič
Mentor: prof. dr. Andrej Petrič
Sinteza in karakterizacija novih fluorescentnih derivatov naftalena
Datum zagovora: 5. 9. 2008

Dragana Kantar
Mentorica: doc. dr. Helena Prosen
Somentor: prof. dr. Samo Kreft
Identifikacija in kvantifikacija sestavin arome ajde (*Fagopyrum esculentum* Moench) z GC-MS
Datum zagovora: 14. 2. 2008

Jakob Kljun
Mentor: prof. dr. Iztok Turel
Koordinacijske spojine rutenija s histaminom in nekaterimi drugimi ligandi
Datum zagovora: 8. 9. 2008

Igor Kovšca
Mentor: prof. dr. Primož Šegedin
Sinteza in karakterizacija koordinacijskih spojin bakra s 4-hidroksipiridinom
Datum zagovora: 16. 10. 2008

Matic Lozinšek
Mentor: prof. dr. Alojz Demšar
Somentor: prof. dr. Boris Žemva
Sinteza in karakterizacija ksenonovih(II) heksafluoromanganatov(IV)
Datum zagovora: 15. 9. 2008

Darja Maučec
Mentor: prof. dr. Anton Meden
Vgradnja mangana v zeolit silikalit-1
Datum zagovora: 13. 6. 2008

Katja Nedižavec
Mentorica: prof. dr. Lucija Zupančič-Kralj
Primerjava ločevanja nekaterih spojin s tenkoplastno kromatografijo v različnih kadeh
Datum zagovora: 10. 7. 2008

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Mentorica: prof. dr. Lucija Zupančič-Kralj
Razgradnja kloriranih spojin z glivami bele trohnobe
Datum zagovora: 28. 3. 2008

Mateja Novak
Mentorica: prof. dr. Brigita Lenarčič
Kloniranje in izražanje fragmentov SMOC-2
Datum zagovora: 14. 4. 2008

Mija Osolnik
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Optimizacija ekstrakcije nekaterih antioksidantov iz sadja
Datum zagovora: 4. 4. 2008

Vesna Papež
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Elektrokemijsko nanašanje magnetnih tankih plasti CoPt-zlitin
Datum zagovora: 17. 12. 2008

Klemen Pirnat
Mentor: akademik prof. dr. Branko Stanovnik
Pretvorbe dietil 1,3-acetondikarboksilata v substituirane piridin-2(1*H*)-one
Datum zagovora: 8. 9. 2008

Tamara Sajevic
Mentor: doc. dr. Jurij Reščič
Vpliv velikosti protiiona na lastnosti raztopin nabitih oligomerov
Datum zagovora: 18. 7. 2008

Natalija Senčar
Mentorica: doc. dr. Saša Petriček
Kompleksi lantanoidnih halogenidov z dietilenglikol dietil etrom in tetrahidrofuranom
Datum zagovora: 25. 1. 2008

Simona Strašek
Mentor: prof. dr. Peter Bukovec
Karakterizacija alumosilikatov na kmetijski zemlji do globine 90 cm
Datum zagovora: 29. 10. 2008

Bine Šebez
Mentor: prof. dr. Marjan Veber
Kronopotenciometrično in voltametrično določevanje arzena v vodah
Datum zagovora: 24. 9. 2008

Karin Šrimpf
Mentor: doc. dr. Bojan Kozlevčar
Koordinacijske spojine kobalta in železa z vanilinom
Datum zagovora: 17. 12. 2008

Andreja Štritof
Mentorica: doc. dr. Helena Prosen
Somentor: prof. dr. Samo Kreft
Primerjava topil pri parni destilaciji z ekstrakcijo ajde
Datum zagovora: 3. 11. 2008

Irena Šutar
Mentor: prof. dr. Boris Pihlar
Določanje nekaterih biološko pomembnih snovi s HPLC in fotometrično ter elektrokemijsko detekcijo
Datum zagovora: 27. 8. 2008

Urška Ulčar
Mentor: prof. dr. Boris Pihlar
Študij interakcij med železom(III) in fitatom
Datum zagovora: 5. 6. 2008

Petra Uršnik
Mentor: akademik prof. dr. Vito Turk
Cepitev in lokalizacija proteina MAGI-3 med apoptozo
Datum zagovora: 19. 9. 2008

Mateja Zupan
Mentor: prof. dr. Janez Plavec
Somentor: doc. dr. Janez Mavri
Izračun reaktivnosti kloroetilen oksida pri alkiliranju DNK
Datum zagovora: 16. 7. 2008

Mojca Zupančič
Mentor: prof. dr. Marjan Veber
Določanje fluorida v nekaterih dodatkih za beton
Datum zagovora: 22. 12. 2008

Andrej Žnidaršič
Mentor: doc. dr. Miran Gaberšček
Sinteza cink fosfatnih nanodelcev za vezavo in kontrolirano sproščanje modelnih proteinov
Datum zagovora: 9. 9. 2008

Martina Žugelj
Mentor: akademik prof. dr. Branko Stanovnik
Sinteze in transformacije substituiranih 3-(dimetilamino)-2-tiazolilpropenoatov
Datum zagovora: 26. 3. 2008

Emanuela Žunkovič
Mentorica: doc. dr. Amalija Golobič
Somentor: prof. dr. Venčeslav Kaučič
Sinteza in strukturna karakterizacija poroznih manganovih karboksilatov
Datum zagovora: 19. 12. 2008

KEMIJSKO IZOBRAŽEVANJE

Petra Apat
Mentor: prof. dr. Boris Pihlar
Določanje saharina in njegovih razkrojnih produktov v elektrolitu za nikljanje
Datum zagovora: 31. 1. 2008

Maja Arzenšek
Mentor: doc. dr. Darko Dolenc
Sinteza analogov in derivatov kurkumina
Datum zagovora: 14. 8. 2008

BIOKEMIJA

Nina Erčulj
Mentor: doc. dr. Marko Dolinar
Priprava prilagodljivega ekspresijskega vektorja pMD203 na osnovi sinteznobiološkega klonirnega vektorja pSB1AC3
Datum zagovora: 12. 6. 2008

Nina Frančič
Mentor: prof. dr. Peter Bukovec
Kovinski kompleksi z glukozaminom
Datum zagovora: 13. 5. 2008

Petra Kaferle
Mentor: prof. dr. Igor Križaj
Somentor: doc. dr. Uroš Petrovič
Razvoj bioinformatske podpore za visoko-zmogljivostne genetske eksperimente: uporaba na primeru valprojske kisline
Datum zagovora: 10. 6. 2008

Vesna Kancilija
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Vpliv cianidnih ionov na anaerobno razgradnjo glukoze
Datum zagovora: 27. 8. 2008

Barbara Koklič
Mentor: prof. dr. Matic Legiša
Vpliv specifičnih vnesenih genov glive *Aspergillus niger* na produkcijo itakonske kisline pri glivi *Aspergills terreus*
Datum zagovora: 23. 4. 2008

Janez Kokošar
Mentor: prof. dr. Igor Križaj
Somentor: doc. dr. Uroš Petrovič
Določanje genetskega interaktoma glavnega regulatorja proliferacije peroksisomov pri kvasovki *S. cerevisiae*
Datum zagovora: 20. 6. 2008

Anja Korenčič
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Termodinamska stabilnost regulatorja bakterijske celične smrti MazG
Datum zagovora: 27. 5. 2008

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Koordinacijske spojine ksanturinske kisline in paladija.
Datum zagovora: 10. 1. 2008

Tina Lahajnar
Mentor: prof. dr. Radovan Komel
Heterologno izražanje transkripcijskih faktorjev družin SREBP in CREM v E. coli in določanje njihove koncentracije v tkivih poskusnih mišk
Datum zagovora: 19. 12. 2008

Kaja Lotrič
Mentor: prof. dr. Matic Legiša
Opis post-translacijske modifikacije encima 6-fosfofrukto-1-kinaze v sesalčjih celicah
Datum zagovora: 15. 9. 2008

Nina Prezelj
Mentorica: doc. dr. Kristina Gruden
Vpliv obrambnih mehanizmov krompirja na razmnoževanje in širjenje virusa PVY^{NTN} po rastlini
Datum zagovora: 29. 2. 2008

Anja Pucer
Mentor: prof. dr. Igor Križaj
Vpliv amoditoksina, fosfolipaze A2 iz strupa modrasa, na mitohondrije modelne celične linije PC12
Datum zagovora: 28. 8. 2008

Igor Škrjanec
Mentor: prof. dr. Matic Legiša
Produkcija bioplina iz pivskih tropin: ugotavljanje metanogenenega potenciala in analiza mikrobne združbe v anaerobni metanogeni biomasi
Datum zagovora: 29. 10. 2008

Marko Šnajder
Mentor: prof. dr. Radovan Komel
Dvodimenzionalna diferenčna gelska elektroforeza v preiskavi adenokarcinoma želodca
Datum zagovora: 12. 9. 2008

Lina Šolmajer
Mentor: doc. dr. Marko Dolinar
Optimizacija izražanja in izolacija rekombinantnih domen transaktivatorja molekul poglavitnega histokompatibilnostnega kompleksa razreda II (CIITA)
Datum zagovora: 24. 12. 2008

Marko Trajkovski
Mentor: prof. dr. Janez Plavec
Študij interakcij kationov z DNA aptamerom trombina
Datum zagovora: 16. 7. 2008

Nina Trošt
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Vloga glivnega sistema ligninolitičnih encimov pri razbarvanju sintetičnih barvil
Datum zagovora: 20. 6. 2008

Tomaž Vargazon
Mentorica: prof. dr. Lucija Zupančič-Kralj
Primerjava ekstrakcijskih postopkov za izolacijo nekaterih kloriranih spojin iz maščob
Datum zagovora: 13. 6. 2008

KEMIJSKO INŽENIRSTVO

Ana Antončič
Mentorica: doc. dr. Urška Šebenik
Vpliv sulfoniranja na sintezo melaminsko – formaldehidnih smol
Datum zagovora: 27. 10. 2008

Boris Bergant
Mentor: prof. dr. Matjaž Krajnc
Vpliv tehnoloških parametrov dispergiranja na kolorističnе lastnosti pigmenta Paliogen Red L 3885
Datum zagovora: 16. 10. 2008

Martina Bošnjak
Mentor: prof. dr. Matjaž Krajnc
Optimizacija sinteze inhibitorja alfa a adrenergičnih receptorjev
Datum zagovora: 13. 3. 2008

Tanja Dobovičnik
Mentorica: doc. dr. Andreja Žgajnar Gotvajn
Korelacije med produkti zgorevanja goriv v Ljubljanski kotlini
Datum zagovora: 17. 12. 2008

Dušan Justin
Mentorica: doc. dr. Andreja Zupančič Valant
Formulacija zračno sušečega premaza na osnovi reoloških lastnosti
Datum zagovora: 22. 1. 2008

Klavdija Krmelj
Mentor: prof. dr. Matjaž Krajnc
Možnosti skladiščenja ogljikovega dioksida v sloj premoga
Datum zagovora: 1. 12. 2008

Robert Matković
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Razvoj mikrostrukturnih naprav z nekovencionalnimi tehnikami
Datum zagovora: 24. 9. 2008

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Mentor: prof. dr. Janvit Golob
Tehnologija praškastih insekticidov
Datum zagovora: 23. 9. 2008

Rok Pirnat
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Kinetični model peroksidne vulkanizacije na pilotni stiskalnici
Datum zagovora: 1. 12. 2008

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Bioremediacija odpadnih vod avtocestnega sistema
Datum zagovora: 26. 5. 2008

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Tehnologija železovega kompleksa z EDTA.
Datum zagovora: 3. 7. 2008

Tina Razboršek
Mentorica: prof. dr. Jana Zagorc Končan
Vpliv odpadnih vod na nitrifikacijsko sposobnost aktivnega blata
Datum zagovora: 17. 7. 2008

Brigita Sever
Mentor: prof. dr. Matjaž Krajnc
Študij prenosa toplote v elastomerih
Datum zagovora: 13. 3. 2008

Tina Skalar
Mentor: doc. dr. Marjan Marinšek
Sinteza materialov za enoprostorsko visokotemperaturno gorivno celico in njena konstrukcija
Datum zagovora: 4. 9. 2008

Tina Šetinc
Mentor: doc. dr. Marjan Marinšek
Električna prevodnost porozne LSM keramike
Datum zagovora: 12. 5. 2008

Jana Štromajer
Mentor: prof. dr. Aleksander Pavko
Razgradnja različnih barvil z bazidiomicetno glivo *Dichomitus squalens*
Datum zagovora: 15. 2. 2008

Tomaž Štrukelj
Mentor: doc. dr. Marjan Marinšek
Vpliv dopantov na poogljičenje Ni-YSZ kompozitov
Datum zagovora: 14. 5. 2008

KEMIJSKA TEHNOLOGIJA

Tomaž Berginc
Mentor: prof. dr. Matjaž Krajnc
Poliedrični oligomerni silseskvioksani kot aditivi za izboljšanje površinskih lastnosti polimernih veziv
Datum zagovora: 19. 2. 2008

Klemen Birtič
Mentor: prof. dr. Aleksander Pavko
Priprava fermentacijske brozge z namenom optimizacije membranskih separacijskih procesov
Datum zagovora: 14. 2. 2008

Suzana Blagojević
Mentor: doc. dr. Franci Kovač
Študij vpliva kisika na stabilnost enocianina in β-karotena v stekleni in PET embalaži
Datum zagovora: 7. 3. 2008

Špela Blatnik
Mentor: prof. dr. Alojz Demšar
Karboksilati prehodnih kovin in lantanoidov
Datum zagovora: 29. 5. 2008

Petra Bric
Mentor: prof. dr. Aleksander Pavko
Encimske aktivnosti med gojenjem glive *Irpex lacteus* na različnih nosilcih
Datum zagovora: 11. 7. 2008

Maša Burjak
Mentor: doc. dr. Urška Šebenik
Določanje vsebnosti trdnih nečistoč v srednjih destilatih in proučevanje vpliva njihove vsebnosti na zmožnost prečrpavanja pogonskega goriva
Datum zagovora: 18. 11. 2008

Katarina Črnič
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Preprečevanje izluževanja ekstraktivnih substanc iz lesa
Datum zagovora: 9. 6. 2008

Leon Dujnko
Mentor: prof. dr. Aleksander Pavko
Izolacija farmacevtskih učinkovin iz organskih topil z nanofiltracijo
Datum zagovora: 25. 9. 2008

Leon Emeršič
Mentor: doc. dr. Marjan Marinšek
Termična analiza citratno – nitratnih gelov
Datum zagovora: 10. 4. 2008

Mojca Erjavšek
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Razvoj vodorazredčljivega premaza za industrijsko obdelavo lesa
Datum zagovora: 6. 3. 2008

Breda Gramc
Mentorica: doc. dr. Helena Prosen
Somentorica: dr. Jana Kolar, viš. znan. sodel.
Uporaba kromatografske metode za določanje molske mase celuloze iz tekstilij
Datum zagovora: 29. 9. 2008

Petra Igličar
Mentorica: doc. dr. Andreja Žgajnar Gotvajn
Postopki zmanjševanja strupenosti v deponijskih izcednih vodah
Datum zagovora: 1. 2. 2008

David Jakše
Mentor: prof. dr. Anton Meden
Uporaba visokotemperaturne rentgenske praškovne difrakcije za karakterizacijo zdravilnih učinkovin
Datum zagovora: 18. 12. 2008

Sanja Jovičić
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Optimizacija adhezivnih lastnosti mikrosfernih akrilatnih lepil
Datum zagovora: 19. 2. 2008

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Globinska in membranska filtracija CHO celične kulture
Datum zagovora: 25. 9. 2008

Petra Kljun
Mentorica: doc. dr. Nataša Gros
Določanje etanola v nizkih koncentracijah z modificirano Conway-evo mikrodifuzijsko celico
Datum zagovora: 30. 6. 2008

Renata Kutnjak
Mentorica: doc. dr. Helena Prosen
Izolacija UDP-MurNAc-L-Alanina-D-glutamata iz reakcijske zmesi encimske reakcije
Datum zagovora: 4. 6. 2008

Rok Lipar
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Nizkocenovna izdelava mikrokanalov
Datum zagovora: 11. 7. 2008

Veronika Ljevar
Mentor: prof. dr. Marjan Veber
Določanje nekaterih elementov v kameni volni z rentgensko fluorescenčno spektrometrijo
Datum zagovora: 11. 7. 2008

Tine Marolt
Mentor: prof. dr. Igor Plazl
Optimizacija porabe premaznih mešanic pri proizvodnji papirja
Datum zagovora: 9. 12. 2008

Sabina Matjašič
Mentorica: doc. dr. Saša Petriček
Kompleksi lantanoidnih halogenidov s polietri in alkoholi
Datum zagovora: 5. 3. 2008

Marjeta Menart
Mentor: prof. dr. Marijan Kočevar
Etil vinil eter kot učinkovit dienofil za cikloadicijske reakcije na 2*H*-piran-2-onih
Datum zagovora: 15. 2. 2008

Eva Munih
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Mikrokapsule
Datum zagovora: 6. 2. 2008

Manja Ocepek
Mentor: doc. dr. Franci Kovač
Priprava substituiranih N-(feniletiliden) anilinov
Datum zagovora: 10. 1. 2008

Petra Olovec
Mentor: prof. dr. Marjan Veber
Vrednotenje metode določanja lahko sprostljivega cianida v odpadnih vodah
Datum zagovora: 6. 6. 2008

Mirjam Peklar
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Sinteza in karakterizacija spojin titana in cirkonija s ciklopentadienilnimi in ciklooktatetraendiilnimi ligandi
Datum zagovora: 18. 12. 2008

Rok Petrič
Mentorica: doc. dr. Andreja Žgajnar Gotvajn
Problematika kovin v izcedni vodi regionalne komunalne deponije
Datum zagovora: 16. 6. 2008

Nataša Polutnik
Mentor: prof. dr. Jadran Maček
Priprava in karakterizacija bakrovega kermeta s cirkonijevim dioksidom
Datum zagovora: 30. 6. 2008

Branka Premrl
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Formuliranje brezbarvne in bele baze za dvokomponentne vodne radiacijsko utrjujoče lesne premaze
Datum zagovora: 15. 7. 2008

Maja Progar
Mentor: doc. dr. Matevž Pompe
Spektrofotometrično določevanje ostankov detergenta po vzorčenju različno dimenzioniranih površin
Datum zagovora: 18. 12. 2008

Urška Resnik
Mentorica: doc. dr. Helena Prosen
Validacija HPLC analizne metode za določevanje zdravilne učinkovine v humani plazmi
Datum zagovora: 16. 12. 2008

Anita Rifelj
Mentorica: doc. dr. Nataša Gros
Validacija HPLC metode za določevanje vsebnosti polimiksina v fermentacijskih brozgah
Datum zagovora: 29. 9. 2008

Jasna Sepaher
Mentor: prof. dr. Marjan Veber
Optimiranje analizne metode za določevanje nekaterih aromatskih ogljikovodikov v zemlji
Datum zagovora: 18. 11. 2008

Špela Smrkolj
Mentorica: doc. dr. Klementina Zupan
Karakterizacija mikrostrukture zlitin v sistemu železo-ogljik
Datum zagovora: 6. 10. 2008

Simon Srpčič
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Porazdelitev elektromagnetnega polja v mikrovalovnem pretočnem cevnem reaktorju
Datum zagovora: 6. 10. 2008

Aleš Škufca
Mentorica: doc. dr. Helena Prosen
Optimizacija ločevanja organskih nepolimernih komponent kavčukovih zmesi s preparativno tekočinsko kromatografijo
Datum zagovora: 27. 8. 2008

Martina Tekavec
Mentor: doc. dr. Andrej Pevec
Sinteza in karakterizacija nekaterih heksafluorometalatov
Datum zagovora: 15. 10. 2008

Andrej Ucman
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Vpliv mikrostrukture kermeta Ni-YSZ na obliko deponiranega ogljika
Datum zagovora: 23. 10. 2008

Tadeja Vidmar
Mentorica: doc. dr. Nataša Gros
Ionsko kromatografska določitev sestave morske vode
Datum zagovora: 18. 12. 2008

Petra Vukovič
Mentorica: doc. dr. Saša Petriček
Sinteza kompleksov lantanoidnih bromidov in kloridov
Datum zagovora: 28. 10. 2008

Tina Žnidaršič
Mentorica: doc. dr. Nataša Gros
Spektrometrično določanje nitrita v odpadnih vodah
Datum zagovora: 4. 6. 2008

Jasmina Žnidaršič
Mentorica: doc. dr. Nataša Gros
Določanje anionov v tehnološki vodi sekundarne strani hladilnega sistema jedrskega reaktorja
Datum zagovora: 28. 11. 2008

VARSTVO PRI DELU IN POŽARNO VARSTVO

Ernest Bahtić
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Varno delo v atmosferah, kjer je prisoten ogljikov oksid
Datum zagovora: 16. 10. 2008

Miha Bergant
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Somentor: pred. mag. Aleš Jug
Osebna varovalna oprema enot civilne zaščite
Datum zagovora: 17. 7. 2008

Dalibor Crljenković
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Revizija postopka odstranjevanja azbesta iz tirnih vozil
Datum zagovora: 18. 12. 2008

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Gasilec potapljač (postopki reševanja iz vode)
Datum zagovora: 28. 3. 2008

Urban Dornik
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Čiščanje komunalnih odpadnih vod v tekstilnem podjetju
Datum zagovora: 20. 3. 2008

Tomaž Gaber
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Varnost pri stroju za globoko vrtanje
Datum zagovora: 21. 5. 2008

Ančka Gantar
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Uvajanja standarda OHSAS 18001
Datum zagovora: 19. 6. 2008

Jasmina Gobec
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Požarna varnost v cestnih predorih
Datum zagovora: 19. 6. 2008

Zlatko Gomilšek
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Somentorica: viš. pred. mag. Barbara Novosel
Nov pristop k vzdrževanju drogov javne in cestne razsvetljave
Datum zagovora: 20. 3. 2008

Jernej Homar
Mentorica: prof. dr. Marija Bešter Rogač
Somentor: prof. dr. Marjan Bilban
Ukrepi za zagotavljanje varnega dela s kremenovim peskom
Datum zagovora: 17. 7. 2008

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Somentorica: viš. pred. mag. Barbara Novosel
Izbor ustreznega sprinklerskega sistema za visoko regalno skladišče Belinka
Datum zagovora: 20. 3. 2008

Maja Jakič
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Analiza varnosti stiskalnic
Datum zagovora: 17. 7. 2008

Peter Jeromel
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Opis poklica gorskega vodnika z vidika varnosti in zdravja pri delu
Datum zagovora: 21. 5. 2008

Iztok Južnič Zonta
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Zahteve požarne varnosti v starih mestnih jedrih
Datum zagovora: 21. 5. 2008

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Meritve in sanacija hrupa pri dveh strojih v podjetju Kovinoplastika Lož d.d.
Datum zagovora: 19. 6. 2008

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Alkoholizem in delovno okolje
Datum zagovora: 6. 6. 2008

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Izračun časa evakuacije iz trgovine
Datum zagovora: 18. 4. 2008

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Usposabljanje delavcev za varno delo v telekomunikacijski družbi
Datum zagovora: 6. 6. 2008

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Posredovanje enot glede na ogroženost Slovenije za naravne in druge nesreče
Datum zagovora: 17. 7. 2008

Jožica Lamovšek
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Ergonomska ureditev embalerske delavnice v Trimu d.d.
Datum zagovora: 28. 3. 2008

Martin Levičar
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Presoja vplivov na okolje za večnamenski prostor – sejmišče
Datum zagovora: 18. 12. 2008

Branko Merlak
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Osebna varovalna oprema v gradbeništvu
Datum zagovora: 4. 12. 2008

Janez Miklič
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Navodila za izbor in uporabo termo IR kamere za namene gasilskih operacij
Datum zagovora: 21. 5. 2008

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Varnost osebnih dvigal in dvigal za gasilce v praksi
Datum zagovora: 17. 7. 2008

Gregor Naglič
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Imisije in hrup pri dveh tipih križišč v Celju ter primerjava v Ljubljani
Datum zagovora: 17. 7. 2008

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Datum zagovora: 19. 6. 2008

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Datum zagovora: 18. 4. 2008

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Datum zagovora: 16. 10. 2008

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Datum zagovora: 16. 10. 2008

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Emisije v lesni in kovinski industriji
Datum zagovora: 16. 10. 2008

Primož Prosen
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Datum zagovora: 16. 10. 2008

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Problematika čiščenja komunalnih odpadnih vod v občini Kočevje
Datum zagovora: 28. 3. 2008

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Promocija prostovoljne privolitve in upravljanje tveganj na področju vzd
Datum zagovora: 4. 12. 2008

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Otroci in vaja evakuacije
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Postavitev sistema ISO 14001 v manjše podjetje
Datum zagovora: 18. 4. 2008

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Varnostni načrt rednega vzdrževanja avtocest v RS
Datum zagovora: 6. 6. 2008

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Razgradnja izrabljenih motornih vozil
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Suhomontažni sistemi v gradbeništvu in njihov vpliv na varnost
Datum zagovora: 4. 12. 2008

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Posredovanje gasilcev ob prometnih nezgodah
Datum zagovora: 18. 12. 2008

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Testiranje zaščitnih sredstev policistov specialne enote Generalne policijske uprave
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Datum zagovora: 21. 5. 2008

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Smernice za izdelavo požarnega načrta
Datum zagovora: 17. 7. 2008

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Povezljivost slovenskih predpisov na področju požarne varnosti
Datum zagovora: 6. 6. 2008

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Analiza poškodb v trgovski družbi
Datum zagovora: 17. 7. 2008

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Zagotavljanje operativnega delovanja gasilskih enot na podeželju
Datum zagovora: 4. 3. 2008

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Standardni operativni postopki ob intervenciji
Datum zagovora: 4. 3. 2008

MAGISTERIJI

KEMIJA

Urška Jerman
Mentor: prof. dr. Marjan Veber
Raziskave matričnih vplivov pri določanju kovin v anorganskih fosfatih z atomsko emisijsko spektroskopijo z induktivno sklopljeno plazmo
Datum zagovora: 2. 4. 2008

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Mentor: viš. znan. sod. dr. Božidar Ogorevc
Somentor: prof. dr. Boris Pihlar
Priprava in karakterizacija glukoznih biosenzorjev na osnovi modificiranih ogljikovih elektrod
Datum zagovora: 7. 4. 2008

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Mentorica: doc. dr. Nataša Gros
Prispevek k predanaliznemu nadzoru kakovosti vakuumiranih epruvet
Datum zagovora: 22. 10. 2008

Simon Makuc
Mentorica: prof. dr. Lucija Zupančič-Kralj
Razvoj analizne metode za določevanje glutationa v iglicah norveške smreke *Picea abies*
Datum zagovora: 14. 11. 2008

KEMIJSKO INŽENIRSTVO

Jošt Mohorko
Mentor: prof. dr. Matjaž Krajnc
Kinetika sinteze in zamreževanja melaminsko-formaldehidnih smol
Datum zagovora: 23. 5. 2008

MATERIALI

Jerneja Godnjavec
Mentorica: prof. dr. Marija Kosec
Vpliv pogojev sinteze na fazno sestavo, mikrostrukturo in električne lastnosti keramike $(K_{0,5}Na_{0,5})NbO_3$
Datum zagovora: 23. 6. 2008

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Predelava in uporaba odpadnega akrilatno / poliestrskega kompozita
Datum zagovora: 23. 6. 2008

INTERDISCIPLINARNI PODILPOMSKI ŠTUDIJ VARSTVO OKOLJA

Sintija Antončič
Mentor: prof. dr. Marjan Veber
Spremljanje nivojev težkih kovin pri kompostiranju mešanice odpadnega blata in micelarne pogače
Datum zagovora: 27. 3. 2008

Nevenka Cukjati
Mentor: prof. dr. Milenko Roš
Somentor: prof. dr. Aleksander Pavko
Primerjalno kompostiranje mezofilno in termofilno stabiliziranega blata iz komunalne čistilne naprave
Datum zagovora: 23. 10. 2008

DOKTORATI

KEMIJA

Monika Inkret
Mentor: prof. dr. Jure Zupan
Merjenje izotopskega razmerja in določanje molske mase silicija z masno spektrometrijo izotopskega razmerja
Datum zagovora: 13. 3. 2008

Martin Tine Perger
Mentorica: prof. dr. Marija Bešter Rogač
Termodinamika micelizacije ionskih in neionskih površinsko aktivnih snovi z različno dolžino polarnega ali nepolarnega dela molekule
Datum zagovora: 14. 3. 2008

Boštjan Jerman
Mentorica: prof. dr. Ksenija Kogej
Termodinamične lastnosti vodnih raztopin izotaktične polimetakrilne kisline
Datum zagovora: 14. 3. 2008

Lidija Pezdirc
Mentor: prof. dr. Jurij Svete
Stereoselektivne in regioselektivne sinteze bicikličnih pirazolidinonov
Datum zagovora: 18. 3. 2008

Marija Meleh
Mentorica: prof. dr. Lucija Zupančič-Kralj
Razvoj in uporaba analizne metode za določanje lizofosfatidne kisline kot označevalca tumorja na jajčniku
Datum zagovora: 21. 3. 2008

Igor Pravst
Mentor: prof. dr. Marko Andrej Zupan
Somentor: znan. svet. dr. Stojan Stavber
Vpliv reakcijskih pogojev na transformacije organskih molekul z *N*-halogeno reagenti
Datum zagovora: 4. 4. 2008

Jernej Wagger
Mentor: akademik prof. dr. Branko Stanovnik
α,β-Nenasičene-α-aminokisline v sintezi nekaterih naravnih spojin in njihovih analogov
Datum zagovora: 7. 4. 2008

Tina Bunič
Mentor: prof. dr. Boris Žemva
XeF_2 in polihidrogenfluoridni anioni kot ligandi v spojinah nekaterih kovinskih(II) heksafluorometalatov in heksafluorofosfatov
Datum zagovora: 9. 4. 2008

Rožle Jakopič
Mentorica: znan. sod. dr. Ljudmila Benedik
Somentor: prof. dr. Boris Pihlar
Analizne metode za določanje izotopskih razmerij uranovih in plutonijevih radioizotopov
Datum zagovora: 11. 4. 2008

mag. Tjaša Urbič
Mentor: znan. sod. dr. Franc Avbelj
Somentor: prof. dr. Vojko Vlachy
Stabilnost fragmentov proteina G
Datum zagovora: 16. 5. 2008

Saša Kovačič
Mentor: prof. dr. Jože Koller
Študij elementarnih reakcij dušikovih oksidov v atmosferskih procesih
Datum zagovora: 18. 6. 2008

mag. Darinka Štajnbaher
Mentorica: prof. dr. Lucija Zupančič-Kralj
Razvoj analizne metode za rutinsko določanje hlapnih pesticidov v živilih
Datum zagovora: 27. 6. 2008

Damjan Šterk
Mentor: prof. dr. Boris Šket
Novi kiralni ligandi za asimetrične redukcije
Datum zagovora: 4. 7. 2008

Maja Gričar
Mentorica: prof. dr. Majda Žigon
Opredelitev kopolimerov asparaginske in mlečne kisline s kromatografskimi metodami in sipanjem svetlobe
Datum zagovora: 16. 10. 2008

Matjaž Mazaj
Mentor: prof. dr. Anton Meden
Somentorica: doc. dr. Nataša Zabukovec Logar
Sinteza in strukturne značilnosti nanoporoznih silikatov in aluminofosfatov
Datum zagovora: 22. 10. 2008

Marija Slavec
Mentor: viš. znan. sod. dr. Božidar Ogorevc
Somentor: prof. dr. Boris Pihlar
Priprava in karakterizacija površinsko modificiranih ogljikovih mikro-elektrod kot senzorjev za nekatere biološko in okoljsko pomembne snovi
Datum zagovora: 17. 10. 2008

mag. Irena Marta Lipar Oštir
Mentor: prof. dr. Ciril Pohar
Termodinamske in transportne lastnosti vodnih raztopin polianetolsulfonske kisline in njenih alkalijskih soli
Datum zagovora: 22. 10. 2008

David Kralj
Mentor: prof. dr. Jurij Svete
Uporaba enaminonov v sintezi pirazolovih derivatov
Datum zagovora: 27. 10. 2008

Uroš Uršič
Mentor: akademik prof. dr. Branko Stanovnik
Novi polifunkcionalni propenoati kot reagenti v sintezi heterocikličnih sistemov
Datum zagovora: 27. 10. 2008

Boštjan Japelj
Mentor: znan. svetnik dr. Boris Orel
Somentor: prof. dr. Matjaž Krajnc
Nanokompozitne hidrofobne, oleofobne in abrazijsko odporne prevleke iz organskih-anorganskih hibridov
Datum zagovora: 28. 10. 2008

Žmitek Katja
Mentor: znan. sod. dr. Jernej Iskra
Somentor: prof. dr. Marko Andrej Zupan
Sinteza, lastnosti in biološke aktivnosti tetraoksanov in sorodnih peroksidnih derivatov
Datum zagovora: 14. 11. 2008

mag. Irena Kozjek Škofic
Mentorica: prof. dr. Nataša Bukovec
Lastnosti tankih plasti cerijevega dioksida in mešanih oksidov cerija z vanadijem in bakrom
Datum zagovora: 21. 11. 2008

Smrkolj Matej
Mentor: prof. dr. Anton Meden
Kristalne strukture in fizikalne lastnosti različnih oblik indapamida in klopidogrelijevega hidrobromida
Datum zagovora: 28. 11. 2008

Tea Zuliani
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Somentorica: prof. dr. Gaetane Lespes
Kritično ovrednotenje analiznih postopkov za speciacijo organokositrovih spojin v vzorcih kopenskega okolja
Datum zagovora: 9. 12. 2008

Peter Brne
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Razvoj CIM nosilcev za afinitetno ločevanje in izolacijo ciljnih proteinov iz krvne plazme
Datum zagovora: 23. 12. 2008

KEMIJSKO INŽENIRSTVO

Jernej Kajtna
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Suspenzijska polimerizacija in sušenje mikrosfernega akrilatnega lepila
Datum zagovora: 14. 4. 2008

mag. Tanja Kurbus
Mentor: viš. znan. sod. dr. Milenko Roš
Somentorica: prof. dr. Jana Zagorc Končan
Razvoj visoko učinkovitega postopka čiščenja odpadnih vod v šaržnem biološkem reaktorju
Datum zagovora: 24. 4. 2008

Sašo Rogelj
Mentor: prof. dr. Matjaž Krajnc
Vpliv procesnih parametrov na reološke lastnosti termoplastičnih polimernih talin med visokotlačnim ekspanzijskim injekcijskim stiskanjem
Datum zagovora: 23. 6. 2008

Blaž Likozar
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Reakcijska kinetika in transportni pojavi med vulkanizacijo elastomerov
Datum zagovora: 22. 10. 2008

MATERIALI

Matjaž Spreitzer
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Vpliv sinteznih in strukturnih značilnosti na električne lastnosti napetostno prilagodljivih materialov na osnovi $Na_{0,5}Bi_{0,5}TiO_3$
Datum zagovora: 10. 3. 2008

RAZISKOVALNI PROGRAMI V OBDOBJU 2004–2008
RESEARCH PROGRAMMES IN THE PERIOD 2004–2008

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 Izr. prof. dr. Matjaž Krajnc	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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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

BIOANORGANSKI SKLOP

Prvi med predvidenimi cilji se nanaša na biomimetske modele interakcij kovinskih ionov z izbranimi organskimi molekulami. Kot kovino smo izbrali molibden, ki je esencialni element in ima vrsto funkcij v živih organizmih. Za molibden v oksidacijskem stanju +5 so značilne $\{Mo_2O_4\}^{2+}$ dinuklearne enote, ki se pri reakcijah z ligandi s kisikovimi donornimi atomi na različne načine samourejajo. Tako smo študirali reakcije piridinijevega hidrogenmaleata z mononuklearnimi oksohalomolibdati. Pripravili smo serijo oksomolibdatnih kompleksov z metanolom, pri čemer pride do nastanka dinuklearnih in tetranuklearnih klastrov. Cis/trans izomerizacija oksomolibdatnih dimerov sodi med osnovne reakcije samourejanja Mo klastrov. Pripravili smo nove komplekse molibdena z malonovo in sukcinsko kislino in jih strukturno karakterizirali.

Naslednji cilj se nanaša na študij vezave kovinskih ionov na biološke makromolekule. Vezava kovinskega iona lahko bistveno spremeni lastnosti makromolekule, pri čemer ima vsak kovinski ion svoj specifični vpliv. Študirali smo koordinacijsko sfero Mn(II), Co(II) in Ni(II) v njihovih kompleksih s hialuronsko kislino, ki smo jih pripravili z reakcijami med Na-hialuronatom in ustreznimi kovinskimi kloridi. S FTIR in EXAFS spektroskopijo smo ugotovili, da je v večini primerov koordinacija kovinskih ionov oktaedrična, redkeje pa tetraedrična. Koordinacijsko število ni odvisno samo od kovinskega iona, temveč tudi od načina priprave

vzorcev. Z molekularnim modeliranjem smo študirali mesta vezave Co(II) na hialuronsko kislino. Posebna pozornost je bila posvečena koordinacijskemu poliedru centralnega atoma, pri čemer smo uporabili kvantnomehansko modeliranje.

Na področju priprave novih Pt(II) kompleksov s citotoksičnim delovanjem so bile raziskave usmerjene v sintezo in izolacijo kompleksov s 3-hidroksimetilpiridinom in 1,7-bis(4-hydroxy-3-methoxy-phenyl)hepta-1,6-diene-3,5-dionom. Karakterizacija spojin je bila narejena predvsem z NMR spektroskopijo in rentgensko strukturno analizo. V sodelovanju z Onkološkim inštitutom je bila določena citotoksičnost naših substanc v primerjavi s citostatiki, ki so v klinični uporabi.

Vloga kovinskih ionov v okolju, posebno v hrani, je zelo aktualna tema, posebno če gre za možne toksične efekte. Znano je, da aluminij povzroča degenerativne poškodbe. Toksičnost je v splošnem odvisna od kemijske zvrsti, pri aluminiju pa zveza med toksičnostjo in tipom zvrsti še ni pojasnjena. Študirali smo speciacijo aluminija v različnih čajnih ekstraktih, tako da smo s kromatografskimi separacijami določili razmerja med posameznimi zvrstmi.

Naslednji cilj predvideva pripravo in študij tankih plasti kovinskih oksidov, ki imajo vrsto potencialnih aplikacij. V seriji treh člankov smo objavili študij sol-gel priprave filmov iz CeO_2 in CeO_2, dopiranega z vanadijevimi oksidi. Dobre elektrokemijske lastnosti pripravljenih filmov smo korelirali z neredom v strukturi filma. V omenjenih treh člankih smo prikazali vlogo termične analize pri optimizaciji elektrokromnega efekta tankih plasti nikljevega oksida, sintetiziranega iz Ni-acetata in Ni-sulfata po sol-gel postopoku. Rezultati kažejo, da imata oba parametra, tako izbrani prekurzor kot tudi režim termične obdelave, bistveni vpliv na elektrokromne lastnosti pripravljenih tankih plasti.

Zadnji cilj predvideva ukvarjanje s problematiko kovin v biološkem in širšem okolju, iskanje specifičnih analiznih rešitev in študij možnosti imobilizacije kovin, ki so v topni obliki in predstavljajo onesnaževanje okolja. Tako smo uvedli metodo za določevanje visokomolekularnih zvrsti aluminija v bioloških vzorcih. Na področju onesnaževanja okolja s kovinami pa smo prikazali možnosti imobilizacije Ni in Zn topnih zvrsti s fosfatnimi stabilizatorji.

BIOORGANSKI SKLOP

Glavni cilj raziskovalnega programa v omenjenem sklopu so nova znanja na področju halogenske organske kemije. Naš poglavitni namen je raziskovanje novih pristopov k selektivni uvedbi halogenskih atomov v organske molekule, tako da pri tem čim bolj posnemamo procese, ki potekajo v naravi. Reagente, substrate in reakcijske pogoje modeliramo tako, da imajo čim večji biomimetski značaj.

Raziskovali smo metode direktnega jodiranja organskih molekul z jodidom ali elementarnim jodom in ugotovili, da je vodikov peroksid v obliki 30 % vodne raztopine ali kompleksa urea/H_2O_2 lahko odličen aktivator teh reakcij, ki hkrati regenerira nastali vodikov jodid v aktiven jodirni reagent, tako da je v večini primerov atomska ekonomija joda maksimalna. Metodologijo smo najprej testirali na vrsti aromatskih molekul pod klasičnimi reakcijskimi pogoji z uporabo organskih topil (metanol, acetonitril), nato pa nadgradili metodologijo, tako da smo za reakcijski medij uporabili vodo ali pa reakcije vodili pod pogoji brez topil. Na osnovi teh odkritij smo take, okolju bolj prijazne sintetske metode, uporabili za selektivno jodiranje alkenov, ketonov in 1,3-dikarbonilnih derivatov. Odkrili in razvili smo tudi metodo aerobnega oksidativnega jodiranja organskih spojih z elementarnim jodom ob prisotnosti $NaNO_2$ kot katalizatorja. Raziskovali smo tudi reakcije bromiranja organskih spojin v vodnem mediju ali

pod reakcijskimi pogoji brez topil z N-bromosukcinimidom (NBS) ali s sistemom HBr/H_2O_2 in ugotovili, da je moč tudi pod temi, okolju bolj prijaznimi pogoji, bromirati ketone in 1,3-dikarbonilne spojine na alfa-mesto ob karbonilni skupini, aromatske molekule pa v odvisnosti od pogojev reakcije na jedro ali benzilno mesto. Prav tako smo uspešno uporabili fluorna topila (npr. perfluorooktan, C_8F_{18}) kot tekočo membrano za počasno in difuzijsko kontrolirano dodajanje broma v reakcijsko zmes, pri čemer se izognemo uporabi kloriranih topil, zmanjšamo količino organskih topil, medtem ko se fluorno topilo v celoti ponovno uporabi brez potrebnega čiščenja. Raziskovali smo reakcije fluoriranja organskih spojin z N-F reagenti v vodi in pod pogoji brez uporabe topil ter ugotovili, da je Selectfluor^{TM} F-TEDA-BF_4 odličen reagent za selektivno fluoriranje v vodnem mediju, medtem, ko je za določene substrate pod pogoji brez topil, boljša izbira reagent NFSi. *Omenjena odkritja pomenijo velik preboj na področju halogeniranja organskih spojin in pomemben prispevek k okolju bolj prijaznemu pristopu pri sintezi organskih molekul. Rezultati omenjenih raziskav so že zelo zgodaj dosegli znatno odmevnost v znanstveni javnosti.*

Pri raziskavah sinteze antimalarijsko aktivnih cikličnih peroksidov smo ugotovili, da uporaba fluoriranih alkoholov kot topil, ki aktivirajo oksidacijske lastnosti vodikovega peroksida, omogoča enostavno in direktno sintezo simetričnih in nesimetričnih 1,2,4,5-tetraoksanov iz enostavnih ketonov, ki smo jim določili tudi antimalarijske aktivnosti in raziskali vpliv polarnosti teh molekul na njihove in vitro aktivnosti. Odkrili smo, da je molekularni jod odličen katalizator za sintezo dihidroperoksidov z direktno okdidacijo ketonov z H_2O_2. *Vsa ta odkritja predstavljajo kvalitativni preskok pri sintezi antimalarikov na bazi cikličnih peroksidov.*

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

BIOINORGANIC CHEMISTRY

Biomimetic models for metal ion interactions with selected organic molecules are one of the goals of the present research. Since it plays an important role in living organisms molybdenum has been selected. When reacting with oxygen donor ligands, molybdenum forms dinuclear $\{Mo_2O_4\}^{2+}$ units in its +5 oxidation state which assemble themselves in specific ways.

Reactions of pyridinium maleate with mononuclear oxohalomolybdates have been studied. A number of oxomolybdate complexes have been prepared with methanol giving binuclear and tetranuclear clusters, and characterised using X-ray diffraction and infrared spectroscopy. Cis/trans isomerisation was shown to be one of the basic reactions in self-assembling Mo clusters. New complexes of molybdenum with anions of malonic and succinic acid have been prepared and structurally characterized.

Further on, we studied the binding of metal ions to biological macromolecules. Such binding can significantly change the properties of macromolecule, with the specific influence of each particular cation. We studied the coordination spheres of Mn(II), Co(II) and Ni(II) in their complexes with hyaluronic acid. It was shown by FTIR and EXAFS that the coordination is usually octahedral, in some cases also tetrahedral. The interaction of Co(II) with hyaluronic acid has been studied, using molecular modeling. Special attention was paid to the evaluation of the coordination polyhedron of the central atom by using quantum molecular modeling.

New Pt(II) complexes of cytotoxic activity have been perpared with 3-hydroxymethylpyridine and 1,7-bis(4-hydroxy-3-methoxy-phenyl)hepta-1,6-diene-3,5-dion and were characterized by NMR spectroscopy and X-ray analysis. Cytotoxicity of prepared complexes was compared with the substances in clinical use.

It is well known that aluminum plays an important role in degenerative diseases. Toxicity of metal ions in the environment, especially in food, is of great importance. Toxicity of an element depends on its speciation in general. The relation between toxicity and speciation for aluminum has not been studied so far. The speciation of aluminum in various tea extracts has been studied by chromatography.

The next goal of the research is to prepare thin films of metal oxides with a number of potential applications. In a series of three articles we have published the results of sol-gel preparation of coatings and characterisation of CeO_2 and CeO_2 doped with vanadium oxides. The comparison of thermal analysis of xerogels and films revealed the applicability of this technique in thin film analysis, developed in our laboratory. Two papers have been published on XANES and EXAFS studies of the afore mentioned films. Good electrochemical properties of these films were correlated with the disorder in their structure. The role of thermal analysis in optimisation of electrochromic effects of nickel oxide thin films using Ni-acetate and Ni-sulphate as precursors has been studied.

The final goal of the project refers to metal ions in biological environment. Soluble aluminum species in food represent a health hazard for humans, where the toxicity may be due to aluminum species present. We introduced an analytical technique for the determination of high-molecular aluminum species in biological samples. Finally, the possibilities of immobilization of soluble Ni and Zn species in the environment, using phosphate stabilization agents have been studied.

BIOORGANIC CHEMISTRY

The main goal of the research is to acquire new knowledge in the field of organohalogen chemistry. Our main scientific interest is to selectively introduce halogen atom into organic compound using biomimetic and ecologically friendly approach.

The methods of direct iodination of organic compounds by using iodides or elemental iodine were investigated, and the effective activation of these reactions using hydrogen peroxide

was discovered. The possibility of performing these reactions also in water media or under solvent-free reaction conditions was established. This new synthetic method was applied in the iodination of a series of organic compounds (alkenes, aromatics, ketones and 1,3-dicarbonyls) and total atom economy for iodine atom was achieved. Aerobic oxidative iodination of organic compounds using molecular iodine in the presence of catalytic amounts of Na_2NO_3 was discovered and developed. We developed a method for radical bromination of alkyl-substituted aromatic compounds by NBS under visible-light activation. We associated fluorous »phase–vanishing« method with visible-light activation for benzylic bromination of organic compounds by bromine. We developed a method for bromination of 1,3-diketones and β–ketoesters using NBS under solvent-free conditions, while only water was used for isolating the products. In the case of aromatic ketones, we could direct regioselectivity by reaction conditions: under solvent-free conditions α-bromination was the exclusive process, while in water, ring functionalisation occurred. Water was used as a reaction medium and H_2O_2/HBr system or NBS illuminated by a 40W incandescent light bulb as a reagent for benzylic bromination of derivatives of toluene. In the case of NBS ring bromination occurred in electron-rich toluenes. With an extensive study of halogenation of organic compounds under solvent-free reaction conditions using N-halosuccinimides we investigated and evaluated crucial parameters which regulate the reaction processes under these conditions. Fluorination of organic compounds with N-F reagents in water or under solvent-free reaction conditions was investigated. Selectfluor™ F-TEDA-BF_4 was found to be an excellent reagent for selective and effective fluorination of organic compounds in aqueous reaction media, while under solvent-free conditions NFSi was found to be a better choice. *These results represent a considerable contribution to modern approaches for the transformation of organic compounds under green reaction conditions.*

We also investigated the synthesis of cyclic tetraoxanes, a new family of potential antimalarian drugs. It was found out that direct transformation of ketones to symetric or asymetric cyclic tetraoxanes is possible by using perfluoro alcohols as a reaction medium, and 30% hydrogen peroxide as an oxidation reagent,. In the compounds obtained we determined antimalaric activities towards *Plasmodium falciparum* and studied the effect of solvent polarity on their in vitro activities. Molecular iodine was found to be a catalyst for direct oxidation of ketones to dihydroperoxides by 30% H_2O_2. *These results represent a considerable contribution to the methodology of synthesizing cyclic tetraoxanes and considerable improvement of current protocols for an efficient preparation of these bioactive materials.*

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 RAZISKOVALNEGA PROGRAMA P1–0153

a) raziskave novih analiznih metod in postopkov,
b) študij procesov in parametrov, ki odločajo o lastnostih anorganskih in organskih materialov,
c) razvoj analiznih metod za meritve v industriji, okolju, medicini in prehrani.

ZNANSTVENI IN DRUGI RELEVANTNI DOSEŽKI

Sodelavci programske skupine so v letih 2004–2008 objavili 104 znanstvene članke, predstavili in objavili raziskovalne dosežke na številnih konferencah, uredili dve monografiji v tujem jeziku, napisali 15 poglavij v znanstvenih monografijah, organizirali tri mednarodna srečanja in en mednarodni simpozij, koordinirali in sodelovali v številnih mednarodnih projektih, izvajali pedagoško delo na dodiplomskem in podiplomskem študiju in bili mentorji 122 diplomantom ter mentorji oz. somentorji 9 magistrandom in 16 doktorandom, razvili tri prototipe instrumentov in prijavili en mednarodni patent, s projekti in raziskavami pa pomembno prispevali k varovanju zdravja in okolja ter k ohranjanju kulturne dediščine. Med pomembnejše dosežke lahko štejemo naslednje:

NEPORUŠNE METODE ZA RAZISKAVE MATERIALOV

Pri kemijski analizi materialov ki predstavljajo predmete kulturne dediščine, sta najbolj kritična odvzem vzorca za analizo in heterogenost sestave tovrstnih materialov. S stališča ohranjanja dediščine je idealna in dopustna le tista tehnika, ki ne zahteva posega v preiskovani material, oz. je stopnja poškodbe pri analizi neznatna. V okviru večletnih raziskav procesov staranja in razgradnje papirja in pisne kulturne dediščine, ki smo jih koordinirali tudi v okviru 5. in 6. OP EU (Papylum, InkCor, SurveNIR, PaperTreat), smo v članku, objavljenem v ugledni reviji *Analytical Chemistry* (JCR IF(2006): 5,646), predstavili nove možnosti za neporušno karakterizacijo in datiranje tovrstnih materialov, kar je svetovna novost. V raziskavi smo z metodo delnih najmanjših kvadratov (PLS) primerjali spektroskopske podatke, pridobljene

v bližnjem in srednjem območju infrardeče svetlobe (FT-IR), z lastnostmi papirja (več kot 170 vzorcev), ki smo jih izmerili s klasičnimi kemijskimi analiznimi metodami. Na ta način smo pokazali, da je možno s FT-IR tehniko na neporušni način izvesti določitev nekaterih ključnih lastnosti kot so vsebnost pepela, lignina, stopnja polimerizacije in pH. Glede na dejstvo, da se ti karakteristični parametri s časom spreminjajo, smo za številne dokumente z izvorom med leti 1650 in 2005 pokazali, da je na osnovi dokaj dobre korelacije med rezultati klasične analize in IR meritev možno tudi neporušno datiranje teh dokumentov (T. Trafela, M. Strlič, J. Kolar, D.A. Lichtblau, M. Anders, D. Pucko, B. Pihlar, Nondestructive analysis and dating of historical paper based on IR spectroscopy and chemometric data evaluation, *Anal. Chem.*, 79(2007)6319–6323; COBISS.SI-ID 28858629). Raziskava predstavlja prispevek k preiskavam zgodovinsko pomembnih materialov in ohranjanju kulturne dediščine.

»PROTIPOVEZOVALNOST«: IZZIV ZA ŠTUDIJ POVEZAV MED STRUKTURO IN LASTNOSTMI KEMIJSKIH SPOJIN

Osnovni problem pri študiju kvantitativnih povezav med strukturo kemijskih spojin in njihovimi lastnostmi (QSPR) oz. aktivnostjo spojin (QSAR), je matematična predstavitev molekularne strukture z ustreznimi deskriptorji. Pogosto srečujemo primere, ko različne funkcionalne skupine v molekuli vplivajo zaviralno ali pa pospeševalno na modelirano lastnost. Do sedaj takih pojavov nismo mogli opisati le z enim matematičnim deskriptorjem, temveč smo uporabljali linearno kombinacijo več strukturnih deskriptorjev. Tako dobljene modele je bilo težko interpretirati. Zaradi tega smo uvedli variabilni »protipovezovalni« indeks, ki istočasno opisuje negativne kot tudi pozitivne vplive posameznih strukturnih delov molekule na njeno modelirano lastnost. Predlagan variabilni povezovalni indeks ničelnega reda je bil prvi matematični opis kemijske strukture, ki je omogočal sočasno opisovanje obeh vplivov z istim deskriptorjem (M. Pompe, Variable connectivity index as a tool for solving the 'anti-connectivity' problem, *Chem. Phys. Lett.*, 404(2005)296-299; COBISS.SI-ID 26572037, JCR IF: 2,438). Uporabnost opisanega strukturnega indeksa smo prikazali na primeru modeliranja faktorjev občutljivosti plamensko ionizacijskega detektorja pri plinski kromatografiji. Kasneje smo za iskanje povezav med strukturo kemijskih spojin ter njihovimi lastnostmi vpeljali še variabilne povezovalne indekse višjega reda z namenom upoštevanja kombiniranega vpliva pozitivnih in negativnih relativnih prispevkov atomov in vezi v strukturi molekule (M. Pompe, M. Randić: "Anticonnectivity": a challenge for structure-property-activity studies, *J. Chem. Inf. Mod.*, 46(2006)2–8; COBISS.SI-ID 27323141, JCR IF: 3,423). Kodirne lastnosti modificiranih indeksov smo preverili na primeru modeliranja reakcijskih hitrosti organskih snovi z OH radikalom v atmosferi. Pri modeliranju smo uporabili variabilni povezovalni indeks prvega reda. Model se je izkazal kot robusten, napaka modela, ki je osnovan na enostavni linearni regresiji pa je znašala 0,343 logaritemske enote. Čeprav je ta napaka višja od tiste, ki smo jo dobili z modeli osnovanimi na multipli linearni regresiji (MLR), je na osnovi tega novega modela mogoče bolje oceniti vpliv posameznih strukturnih komponent na reaktivnost organskih spojin.

KEMILUMINESCENCA – ORODJE ZA ŠTUDIJ RAZGRADNJE CELULOZNIH MATERIALOV

Kemiluminescenca, ki jo pri raziskavah polimernih materialov uporabljajo že vrsto let, se je v novejšem času izkazala kot zelo primerno orodje za raziskave mehanizmov razgradnje celuloze. Raziskave, ki smo jih koordinirali v okviru projekta Papylum (5. OP EU), so pokazale, da poleg temperature na luminescenco papirja pomembno vpliva tudi vsebnost vode v preiskovanem materialu. Da bi lahko izvedli tovrstne meritve smo razvili nov instrument, s katerim lahko poleg temperature in sestave atmosfere med merjenjem kemiluminescence kontroliramo

tudi vlažnost atmosfere ob vzorcu. Rezultati so potrdili, da vsebnost vode pomembno vpliva na razgradnjo celuloze pri temperaturah pod 100 °C, za to pa obstaja več vzrokov. Z eksperimenti pospešene razgradnje smo ugotovili, da je pri 60–80 % RH razgradnja najhitrejša, medtem ko poteka počasneje tako pri nižji kot pri višji relativni vlažnosti, česar si ne moremo razložiti s popravkom za vsebnost vode v atmosferi. Odgovor na to vprašanje smo skušali dobiti z razlago kinetike reakcij razgradnje celuloze v vlažni atmosferi, ki smo jih z razvito instrumentacijo lahko zasledovali s pomočjo dinamičnih meritev kemiluminescence. Eksperimentalni podatki so pokazali, da je superoksidni anion pomemben prekurzor luminescentne zvrsti, za katero menimo, da je singletni kisik. Rezultati teh raziskav so bili med drugim objavljeni v znanstvenem članku (D. Kočar, M. Strlič, J. Kolar, J. Rychlý, L. Matisová-Rychlá, B. Pihlar, Chemiluminiscence from paper III: the effect of superoxide anion and water, *Polym. Degrad. Stab.*, 88(2005)407–414; COBISS.SI-ID 26572549, JCR IF: 1,749), opisani pa so tudi v doktorski disertaciji (COBISS.SI-ID 28554757), ki je bila nagrajena s Samčevo nagrado (FKKT, 2007) in v več poglavjih monografije (COBISS.SI-ID: 219327232, 28510213). Dosežki predstavljajo pomemben doprinos k raziskavam ohranjanja materialov kulturne dediščine.

OBSTOJNOST ZGODOVINSKIH ZAPISOV Z ŽELEZO-GALNIMI ČRNILI

Železo-galna (taninska) črnila se v zahodni civilizaciji pojavljajo vse od srednjega veka naprej in predstavljajo najpomembnejša črnila, s katerimi je zabeleženih tudi večina zgodovinsko pomembnih zapisov. Znano je, da železo in druge kovine, ki jih ta črnila vsebujejo, delujejo na papir korozivno, kar povzroča nezadržen propad teh dokumentov. Vzroke za korozivnost in možnosti za stabilizacijo zgodovinskih dokumentov, ki smo jih raziskovali tudi v okviru evropskih projektov 5. OP EU InkCor in MIP, smo opisali med drugim v raziskavi, objavljeni v reviji Analytica Chimica Acta (JCR IF: 2,894), kjer smo študirali vpliv različnih parametrov na obstojnost železo galnih črnil z veliko vsebnostjo prehodnih kovin in kislin (J. Kolar, A. Štolfa, M. Strlič, M. Pompe, B. Pihlar, M. Budnar, J. Simčič, B. Reissland: Historical iron gall ink containing documents – properties affecting their condition, *Anal. Chim. Acta*, 555(2006)167–174; COBISS.SI-ID 19492391). Ker se je izkazalo, da so nekatera črnila bolj korozivna od drugih, nas je v tej študiji zanimalo, kateri so dejavniki, ki k temu najbolj pripomorejo. Pri delu smo uporabili vrsto analiznih metod, ki smo jih razvili sami, zlasti PIXE (COBISS.SI-ID 19596071), pa tudi potenciometrično določanje pH črnila. S statistično analizo podatkov smo pokazali, da na korozivnost največ vplivajo količina nanosa črnila, pH črnila in gramatura papirja. Na podlagi teh podatkov, ki smo jih večinoma pridobili z neporušnimi metodami, je tako možna napoved stabilnosti zgodovinskih dokumentov, ki so napisani z železo galnim črnilom, kar smo opisali tudi v poglavju monografije (COBISS.SI-ID 28288773). Delo je pomemben prispevek k poznavanju procesov propadanja dokumentov kulturne dediščine.

VISOKO ZMOGLJIVA METODA ZA DOLOČANJE PESTICIDOV

Pesticidi in njihovi razkrojni produkti predstavljajo v okolju in živilih zaradi intenzivne uporabe v agroživilstvu ter številnih interakcij teh snovi v naravi, pomemben ekološki in zdravstveni problem in zahteven analizni izziv. V odmevni raziskavi, ki smo jo objavili v ugledni reviji *Journal of Chromatography* A (članek je uvrščen med 50 najbolj citiranih del te revije v obdobju 2002–2007), smo razvili in optimizirali GC-MS metodo za določanje pesticidov v sadju in zelenjavi (D. Štajnbaher, L. Zupančič-Kralj, Multiresidue method for determination of 90 pesticides in fresh fruits and vegetables using solid-phase extraction and gas chromatography-mass spectrometry, *J. Chromatogr.* A, 1015 (2003)185–198, COBISS.SI-ID 25393925], JCR IF 2,922). Metoda temelji na predpripravi vzorcev z ekstrakcijo pesticidov z acetonom v kom-

binaciji s predkoncentriranjem/čiščenjem z ekstrakcijo na trdno fazo (SPE) in ionsko izmenjavo (IEX). Z optimizacijo postopka priprave vzorcev (ekstrakcija, SPE, IEX), kromatografskih pogojev in MS detekcije (m/z), smo z eno analizo v različnih vrstah sadja in zelenjave, lahko določili do 90 pesticidov hkrati z negotovostjo pod 10 % (RSD). Metodo smo dodatno izpopolnili z uvedbo temperaturno programiranega uparjalnika (PTV), ki omogoča vnos večjega volumna vzorca (10 µL) v GC-MS sistem (D. Štajnbaher, L. Zupančič-Kralj, Optimisation of a programmable temperature vaporizer-based large volume injection for determination of pesticide residues in fruits and vegetables using gas chromatography-mass spectrometry, *J. Chromatogr*. A, 1190(2008)316–326, COBISS.SI-ID 29445381, JCR IF (2006): 3.554). Z miniaturizacijo postopka predpriprave vzorcev z ekstrakcijo na reverzni fazi (RP-SPE), je pri uporabi PTV modula možna sočasna identifikacija in kvantitativna določitev 124 pesticidov. Visoka zmogljivost metode in nizka meja kvantifikacije (0,01 mg/kg) bo omogočala boljše in hitrejše analize in s tem bolj kvalitetno kontrolo prehrambenih artiklov ter na ta način pomembno prispevala k varnosti živil, kar je ena izmed pomembnih prioritet tako v slovenskem kot v svetovnem prostoru.

STARANJE IN STABILIZACIJA PAPIRJA

Raziskave procesov staranja in razgradnje celuloznih vlaknin in papirja so bile tudi del mednarodnega projekta Papylum, 5. OP EU (EVK4-CT-2000-00038), ki ga je koordinirala naša inštitucija, smo poleg številnih objav v znanstveni periodiki strnili v monografiji z naslovom »Staranje in stabilizacija papirja« (*Ageing and stabilisation of paper*, Edited by M. Strlič and J. Kolar, National and University Library, Ljubljana, 2005, ISBN 961-6551-03-5, COBISS.SI-ID 219327232). Monografija, ki je pisana v angleščini in obsega 211 strani, predstavlja zbir najnovejših dosežkov in znanj na področju raziskav o razgradnji celuloze in procesih, ki se dogajajo pri staranju pisne kulturne dediščine. V dvanajstih poglavjih, ki so razdeljena na tri področja: metodologija, degradacija in stabilizacija papirja, so zajeti vsi bistveni procesi in pristopi, ki se danes uporabljajo pri raziskavah, povezanih z razgradnjo papirja. V osmih poglavjih so tudi prispevki sodelavcev programske skupine z rezultati najnovejših raziskovalnih dosežkov na področju analizne metodologije za študij depolimerizacije celuloze, termooksidativne degradacije papirja in strategij za stabilizacijo celuloznih vlaknin (COBISS.SI-ID: 26642693, 26642949, 26643205, 26643461, 26643717, 26643973, 26650373, 26650885). Monografija predstavlja uporaben priročnik tako za raziskovalce kot za konzervatorje in vse, ki skrbijo za ohranitev kulturne dediščine. Raziskovalno delo in dosežki na tej problematiki so uvrstili sodelavce laboratorija in programske skupine med vodilne strokovnjake in svetovno priznane centre na tem področju. Pridobljena znanja iz teh raziskav bodo vključena tudi v nove univerzitetne študijske programe kemije na UL FKKT v okviru predmeta »Karakterizacija in stabilnost materialov kulturne dediščine«.

MEDNARODNI SIMPOZIJ O SEPARACIJSKIH ZNANOSTIH

Sekcija za analizno kemijo pri Slovenskem kemijskem društvu in Avstrijsko združenje za analizno kemijo (Austrian Society for Analytical Chemistry) sta organizirala v septembru 2006 v Lipici 12. mednarodni simpozij o separacijskih znanostih (M. Strlič, (ur.), W. Buchberger (ur.), 12th International Symposium on Separation Sciences, Lipica, Slovenia, September 27th–29th, 2006. Book of abstracts: Lipica 2006. Ljubljana: Slovensko kemijsko društvo, 2006. 356 str. ISBN 961-90731-6-9. ISBN 978-961-90731-6-2, COBISS.SI-ID 228508416). Na simpoziju, ki mu je predsedovala prof. L. Zupančič-Kralj, je sodelovalo 192 udeležencev in je bil daleč najbolj obiskan simpozij v tej vrsti do sedaj. Slovenskih udeležencev je bila le dobra tretjina,

zato lahko rečemo, da je šlo za resnično mednarodni simpozij – znanstveni odbor pa so sestavljali kolegi iz cele Evrope. Predstavljenih je bilo 153 prispevkov, ki so izšli v knjigi povzetkov, prosto dostopnih na internetu, izbrani prispevki pa so bili v okviru znanstvenih člankov v razširjeni obliki objavljeni v tematski številki znanstvene revije *Acta Chimica Slovenica*, v kateri je tako izšlo 22 člankov (COBISS.SI-ID 28517893).

Simpozij je bil velikega pomena tudi za sodelavce iz industrije, saj se jih je udeležilo 45, kar je vzpodbudno število. Na simpoziju je sodelovalo tudi 12 razstavljavcev, hkrati pa smo organizirali tudi dve praktični delavnici, s čimer smo intenzivirali prenos znanja. Simpozij smo organizirali s sofinanciranjem ARRS. Glede na izjemno udeležbo lahko rečemo, da je simpozij uspel in da je tudi izbrana organizacijska shema (predavanja – delavnice – razstava – plakati) primerna ter atraktivna tako za akademsko sfero kot za industrijo. Na simpoziju je bila predstavljena tudi vrsta raziskovalnih dosežkov članov programske skupine, kar je, poleg same organizacije, pomembno prispevalo k promociji dosežkov slovenske znanosti.

NOV POSTOPEK ZA STABILIZACIJO ZGODOVINSKIH DOKUMENTOV

V okviru projekta InkCor, 5. OP EU (EVK4-CT-2001-00049), ki ga je koordinirala J. Kolar, na UL FKKT pa M. Strlič, smo raziskovali korozivnost železo galnih črnil in razvijali metode za stabilizacijo dokumentov in zgodovinskih zapisov s temi črnili. Sodelovanje v projektu lahko označimo kot izjemno uspešno, saj smo poleg številnih objav uredili tudi znanstveno-strokovno monografijo z naslovom »*Iron gall inks: on manufacture, characterisation, degradation and stabilisation*«, National and University Library, Ljubljana, 2006 (ISBN 961-6551-19-1, ISBN 978-961-6551-19-9, COBISS.SI-ID 230700544). Monografija opisuje izvor, sestavo, karakterizacijo in stabilizacijo dokumentov z železo galnimi črnili. V okviru projekta je bil razvit nov tehnološki postopek z uporabo antioksidantov, za katerega je bila podana patentna prijava (COBISS.SI-ID 26939909). Učinkovitost predlaganega postopka smo preverili na množici drugih dokumentov in tudi drugih materialov. Nov izdelek je v obliki tekočine za obdelavo – stabilizacijo na trgu že ponudilo nemško podjetje Zentrum für Bucherhaltung GmbH. V monografiji opisujemo njegovo učinkovitost in evaluiramo stranske pojave. Hkrati so v monografiji poglavja, h katerim so raziskovalci naše programske skupine še posebej pripomogli (COBISS.SI-ID: 28288773, 28289285, 28289797, 28290309, 28290565). Dosežki so pomembni za stabilizacijo in zaščito dokumentov kulturne dediščine in pomembno prispevajo k promociji slovenske znanosti.

MIKROELEKTRODA ZA MERJENJE pH PAPIRJA

Za merjenje pH običajno uporabljamo stekleno elektrodo, ki pa pri papirju ne omogoča merjenja, ne da bi uničili ali poškodovali vzorec. Kot je znano, je pH makromolekulske okolice v papirju eden izmed najbolj pomembnih parametrov, ki definirajo življenjsko dobo papirja. Večina postopkov, ki so danes v uporabi za določanje pH zgodovinskih vzorcev, je neprimernih, med njimi tudi miniaturna steklena elektroda, predvsem zaradi mehanske krhkosti. Zato smo razvili novo robustno elektrodo iz steklastega grafita, na katerega smo s pomočjo elektropolimerizacije nanesli tanko plast polianilina (M. Strlič, B. Pihlar, L. Mauko, J. Kolar, S. B. Hočevar, B. Ogorevc: A new electrode for micro-determination of paper pH, *Restaurator*, 26(2005)159–171; COBISS.SI-ID 3342874). Elektrodo smo testirali na različnih realnih vzorcih in točnost meritev pH s to elektrodo preverili s predpisanimi standardnimi postopki ter dobili dobro ujemanje. Ker se je elektroda pokazala predvsem zaradi nedestruktivnega načina merjenja uporabna, smo izdelali ustrezno stojalo in referenčno Ag/AgCl elektrodo, ki

omogočata enostavno kalibracijo in merjenje pH z minimalno interakcijo oz. poškodbo vzorca pri merjenju. Raziskave smo posvetili tudi študiju interferenc in kalibraciji. Prototip elektrode omogoča merjenje pH neposredno na dokumentu z minimalno omočitvijo vzorca (1–2 µl). Preizkusili smo ga na številnih realnih vzorcih in dobili dobre rezultate in pozitivni odziv pri potencialnih uporabnikih. Razvoj tehničnega prototipa iz laboratorijskega prototipa je deloma potekal v okviru projekta Eureka 3843 in ga nameravamo v bodoče razviti v okviru spin-off podjetja (Morana RTD) v tehnološko uporaben produkt.

HLAPNE ORGANSKE SNOVI V ZRAKU

V okviru večletnih raziskav emisij in transporta hlapnih organskih ogljikovodikov (VOC) v slovenskem prostoru in širše, smo v vabljenem predavanju predstavili pregled analiznih tehnik in aktualnih problemov in dosežkov laboratorija na tem področju. Za določanje VOC in njihovih oksidacijskih produktov v atmosferi najpogosteje uporabljamo plinsko (GC) in tekočinsko kromatografijo (HPLC) z masnospektrometrično detekcijo (MS) in drugimi detektorji. Pri tem naletimo pri teh kompleksnih vzorcih tako na probleme identifikacije, kjer si poleg specifične detekcije z MS pomagamo z numeričnimi pristopi, kot na težave pri kvantifikaciji (nizke koncentracije). Rešitev predstavlja samo dobra separacija v kombinaciji s predkoncentriranjem, ki mora biti tako učinkovito, da omogoča merjenje ekstremno nizkih koncentracij v ppb do ppt območju. V prispevku so bili prikazani nekateri načini določanja značilnih hlapnih organskih snovi antropogenega in biogenega izvora in nekaterih njihovih oksidacijskih razkrojnih produktov s poudarkom na analitskih problemih, predstavljene so bile tudi rešitve. Delo je bilo predstavljeno v okviru vabljenega predavanja in objavljeno v zborniku konference (M. Pompe, M.Veber, Determination of volatile organic compounds in the air, P. Glavič (ur.), D. Brodnjak Vončina (ur.), Slovenski kemijski dnevi 2005, Maribor, 2005; COBISS.SI-ID 27020805) in predstavlja doprinos k zaščiti okolja.

Poleg zgoraj omenjenih dosežkov, navajamo še naslednje:

a) V okviru raziskav povezave med strukturo in lastnostmi spojin smo raziskovali možnosti za napovedovanje termodinamskih količin na osnovi kemijske strukture (COBISS.SI-ID 25800197) in s plinsko kromatografijo uspeli identificirati spojine glede na retencijske lastnosti v homologni seriji *n*-alkanov, 1-alkenov in 2-alkenov. Študirali smo tudi uporabo variabilnih povezovalnih indeksov za napovedovanje reakcijskih hitrosti (COBISS.SI-ID 26342917, COBISS.SI-ID 29915397) in modelirali pK_a vrednosti halogeniranih organskih kislin (COBISS.SI-ID 28928005). Študij razvoja enostavnih matematičnih opisov kemijske strukture smo nadaljevali na primeru benzenoidnih spojin, med katerimi so mnoge kancerogene (COBISS.SI-ID 28508165) in v okviru sodelovanja z uglednimi tujimi raziskovalci razvili metodo za rangiranje posameznih benzenoidov, osnovano na osnovi porazdelitve π elektronov med kondenziranimi obroči (COBISS.SI ID 29447429, COBISS.SI-ID 29976325]).

Raziskovali smo tudi vpliv matričnih sestavin (HNO_3, MeOH) na določanje fosforja z elementno ICP-MS tehniko (COBISS.SI-ID 3386650) ter razvili dva instrumenta in sicer plinski kromatograf (COBISS.SI-ID 1246044]) in spektrofotometrični mikrotitrator (COBISS.SI-ID 25549829, 28579077), ki zaradi preproste konstrukcije in enostavnih sestavnih komponent omogočata uporabo in poučevanje tovrstnih tehnik v šolah. Optimizirali smo pogoje za simultano določitev makro in mikrokomponent v morski vodi in sorodnih vzorcih z ionsko kromatografijo in tako določeno ionsko sestavo vod povezali z drugimi prametri, ki opredeljuje kakovost in značaj vod (COBISS.SI-ID 29873157). Razvijali smo tudi metode tekočinske kromatografije (HPLC) in micelarne elektrokinetične kromatografije (MEKC) za določanje manj hlapnih pesticidov (triazini) in njihovih razkrojnih produktov in jih uporabili za študij

interakcij s huminskimi substancami in nekaterimi mineralnimi snovmi v naravi (COBISS. SI-ID 26061829).

V sodelovanju z industrijo (LEK d.d.) smo razvili hitro kromatografsko metodo za ločbo pravastatina od mevastatina in 6-*epi* pravastatina v fermentacijski brozgi (COBISS.SI-ID 84418). Metoda se odlikuje s kratkim časom analize (1 minuta), ki omogoča učinkovito spremljanje biosinteze te učinkovine v farmacevtski proizvodnji. V sodelovanju s Krko d.d., smo raziskovali parametre, ki vplivajo na sproščanje farmacevtske učinkovine diklofen iz tablet (COBISS.SI-ID 26133765) in s pomočjo faktorske analize opredelili ključne parametre, ki so pomembni za za kinetiko sproščanja te učinkovine iz farmacevtskih formulacij (COBISS.SI-ID 1438577). V sodelovanju s podjetjem BIA smo raziskovali možnosti za uporabo monolitnih kromatografskih nosilcev za hitro izolacijo in delno frakcionacijo proteinov in analize v proteomiki (COBISS.SI-ID 1298268), v sodelovanju s Kemijskim inštitutom pa razvili računalniški model za separacijo anionov z ionsko kromatografijo (COBISS.SI-ID 3858970).

b) V okviru študija procesov stabilnosti in razgradnje organskih materialov smo raziskovali parametre, ki vplivajo na kinetiko depolimerizacije celuloznih vlaknin in papirja ter preučevali korozivnost zgodovinskih črnil in nekaterih drugih materialov (Co in Cu-Zn zlitine). Študirali smo vpliv lastnosti celuloznih vlaknin, kot so kristaliničnost, morfologija in velikost, na kemiluminescenco papirja (COBISS.SI-ID 26156037), s pomočjo ^{13}C-1 markirane glukoze raziskovali oksidacijo končnih skupin na celulozi in kvantitativno razložili fenomen samoabsorpcije svetlobe med merjenjem kemiluminescence papirja (COBISS.SI-ID 29192453). Študirali smo fotooksidacijo celuloze (COBISS.SI-ID 26628357) in raziskovali katalitski vpliv nekaterih halidnih anionov in kovin na Fentonove procese pri oksidativni razgradnji celuloze (COBISS.SI-ID 27068677, 28858373). S pomočjo NIR spektroskopije in kemometrije smo določali mehanske lastnosti zgodovinskih papirjev in izdelali prenosni NIR instrument (COBISS.SI-ID 29804549). Korozivnost železo galnih črnil smo obravnavali v več člankih in predlagali novo analizno metodologijo za ovrednotenje poškodovanih dokumentov (COBISS. SI-ID 214488576). Za ugotavljanje oksidacijskega razmerja med Fe(II) in Fe(III) v zgodovinskih črnilih, ki pomembno vpliva na njihovo korozivnost, smo preučili uporabnost XANES spektroskopije (COBISS.SI-ID 665339). Pokazalo se je, da je za pravilnost rezultatov analize pri tej tehniki bistvena izbira referenčnih spojin. Te morajo imeti enako simetrijo s sosednjimi atomi in enako lokalno strukturo, kot jo imajo originalni vzorci. Z namenom poiskati učinkovit inhibitor, ki bi bil uporaben tudi za aplikacijo in obdelavo zgodovinsko pomembnih zapisov v nevodnem mediju, smo sintetizirali dva mio-inozitol fosfata (COBISS.SI-ID 27520261), ki sta pokazala fitinski kislini podobne inhibitorne lastnosti in s pomočjo ^{31}P NMR in rentgenskih tehnik raziskovali interakcije in strukturo Fe(III) inozitol heksafosfatov (COBISS.SI-ID 3617562). Raziskovali smo značilnosti procesov za stabilizacijo papirja z železo galnimi črnili (COBISS.SI-ID 27066373) in predlagali izboljšave postopka z obdelavo z magnezijevim fitatom (COBISS.SI-ID 29238533) ter raziskovali možnosti za kontrolirano čiščenje papirja in dokumentov z laserjem (COBISS.SI-ID 26905605).

Z obširno raziskavo in kritično presojo obstoječih postopkov za merjenje pH papirja (COBISS.SI-ID 26114309) smo ovrednotili teorijo in eksperimentalne vplive, ki odločajo o točnosti potenciometričnih in kolorimetričnih meritev tega parametra. Na osnovi teh rezultatov in slabosti, ki jih imajo obstoječi standardni postopki, smo izdelali robustno mikroelektrodo iz steklastega grafita, modificiranega s polianilinom (COBISS.SI-ID 3342874), ki omogoča lokalno merjenje pH na dokumentih. Z analizo hlapnih sestavin (VOC), ki se sproščajo med razgradnjo papirja, smo pokazali, da je z nekoliko bolj zahtevno instrumentacijo in postopkom možno tudi popolnoma neporušno določanje pH zgodovinskih dokumentov (COBISS.SI-ID 29134853). Metoda temelji na merjenju emisije furfurala s plinsko kromatografijo sklopljeno

z masno spektrometrijo (GC-MS), saj emitirane koncentracije dobro korelirajo s pH papirja. V okviru raziskav kovinskih materialov smo študirali obstojnost zlitin kobalta v fizioloških medijih (COBISS.SI-ID 17668313, 18268711) in proučevali procese, ki vplivajo na korozijo Cu-Zn zlitin (COBISS.SI-ID 18793255, 19217959).

c) V okviru raziskav povezanih z okoljem, prehrano in biološkimi sistemi, smo raziskovali možnosti za ekstrakcijo nekaterih pesticidov iz tal s pomočjo mikrovalov (COBISS.SI-ID 621526) in študirali kinetiko fotokemijskih pretvorb atrazina in njegovih razgradnih produktov v okolju (COBISS.SI-ID 26342405). Porazdeljevanje in sorpcijo nekaterih izbranih okoljskih onesnaževal (PCB-ji, klorosubstituirani insekticidi, triazinski in amidni herbicidi) na huminske kisline, zemljo in mineralne snovi, smo raziskovali z mikroekstrakcijo na trdno fazo (COBISS.SI-ID 28423173). S pomočjo velikostne izključitvene kromatografije in masne spektrometrije z induktivno sklopljeno plazmo (ICP-MS), smo študirali vezavo kovin na huminske spojine v ekstraktu komposta (COBISS.SI-ID 28522245) in izdelali metodo za določanje selena v rastlinah, osnovano na HPLC-UV-Hg-AFS (COBISS.SI-ID 19685671). Razvili smo metodo za določanje ohratoksina A v vinu, osnovano na on-line ekstrakciji ter HPLC separaciji v kombinaciji s fluorimetrično detekcijo ter s HPLC-MS preučili stabilnost toksina pri dnevni svetlobi (COBISS.SI-ID 27677957). Razvili smo ekstrakcijski postopek za analizo sestavin arome mošta in vina, osnovan na mikroekstrakciji na trdno fazo (DVB/CAR/PDMS vlakno) in identifikaciji/kvantifikaciji z GC-MS in LC-MS (COBISS.SI-ID 4982649, 5326969]). Določevali smo proste aminokisline (AK) v moštih in mladih vinih s pred-kolonsko derivatizacijo primarnih AK s 3-MPA/OPA in sekundarnih AK s FMOC-Cl. Ker imajo ti vzorci zelo različno vsebnost sladkorjev, smo preučevali vpliv sladkorjev na derivatizacijo z uporabo dveh internih standardov: (i) primarno AK norvalinom in (ii) sekundarno AK sarkozinom in sicer v realnih vzorcih ter v modelnih raztopinah fruktoze in glukoze. Opazili smo velik vpliv matrice, še posebno, če je bila koncentracija sladkorjev večja kot 50 g/L (COBISS.SI-ID 29802245).

Raziskovali smo tudi interakcije kinolonskega antibiotika ciprofloksacina z eno in dvovalentnim bakrom (COBISS.SI-ID 1668977) in razvili HPLC-MS/MS analizno metodo za izolacijo lizofosfatidnih kislin (LPA) kot potencialnih biomarkerjev iz plazme (COBISS.SI-ID 2189937). Metodo smo uporabili za določanje LPA v serumih pacientk z različnimi tumorji na jajčnikih (COBISS.SI-ID 23159001). 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.

Furokumarini se naravno pojavljajo v različnih rastlinah, predvsem v raznih vrstah citrusov. Ker imajo številne fiziološke učinke, je potrebno nadzirati njihovo koncentracijo v proizvodih, namenjenih za človeško rabo. Razvili smo LC-MS/MS metodo v kombinaciji z ekstrakcijo na trdno fazo (SPE) za določanje bergaptena in bergamotina v različnih vzorcih pijač in kozmetike. Zaradi izrazitega vpliva matrice je bil najbolj zanesljiv način kvantifikacije metoda standardnega dodatka. (COBISS.SI-ID 29682437).

RESEARCH PROGRAMME REPORT

RESEARCH TOPICS AND GOALS OF THE PROGRAMME P1–0153

a) Research and development of novel analytical methods and procedures,
b) Study of processes and parameters which determine the properties of inorganic and organic materials,
c) Development of analytical methods for industrial applications, medicine, environmental studies and food analysis.

SCIENTIFIC AND OTHER RELEVANT ACHIEVEMENTS

In the period between 2004 and 2008, members of the programme group published 104 original scientific papers, delivered a number of lectures at scientific conferences, edited two scientific monographs, contributed to 15 chapters in scientific monographs, organized three international meetings and one international symposium, coordinated and participated in numerous international scientific projects, developed three prototypes of instruments and applied for one international patent. They were also involved in teaching at undergraduate level (supervised 122 diploma theses) and post-graduate level (supervised and co-supervised nine master and 16 doctoral theses). Participation in projects, as well as research activities contributed to scientific and socio-economic progress in Slovenia in the field of health protection, protection of the environment and preservation of cultural heritage. The following scientific achievements should be emphasised:

NON-DESTRUCTIVE METHODS FOR MATERIALS CHARACTERISATION

In the analysis of heritage materials, sampling represents the most critical aspect of the analytical process, along with material heterogeneity. From the viewpoint of material conservation, only non-destructive material characterisation is allowable – no sampling or sample destruction during analysis is acceptable. The research extended over several years, some of which was part of the 5th and 6th FP EU programme. Projects Papylum, Inkcor, SurveNIR, Paper-Treat resulted in innovative non-destructive methods for historical material characterisation, which were published in the leading journal *Analytical Chemistry* (JCR IF(2006): 5,646). Using the method of partial least squares (PLS), we were able to compare FT-(N)IR spectroscopic data with the results of classical paper analysis of more than 170 samples. We showed that by using the FT-IR technique, it is possible to model ash and lignin content, the degree of polymerisation and pH. Considering the fact that these properties change with time, we were able to date historical paper with considerable certainty. In this research, we used paper dated from 1650–2005 (T. Trafela, M. Strlič, J. Kolar, D.A. Lichtblau, M. Anders, D. Pucko, B. Pihlar, Nondestructive analysis and dating of historical paper based on IR spectroscopy and chemometric data evaluation, *Anal. Chem*., 79(2007)6319–6323; COBISS.SI-ID 28858629). This piece of research contributes considerably to our understanding of heritage materials and their conservation.

"ANTICONNECTIVITY": A CHALLENGE FOR STRUCTURE-PROPERTY-ACTIVITY STUDIES

The central problem in quantitative structure-property (QSPR) or structure-activity (QSPR) studies is how to identify critical structural factors relevant for the variation of different properties. There are several molecular properties where the presence of a certain atom or functional group in the molecule suppresses the observed property. None of the present atom and bond additive topological indices, including variable connectivity indices, when used alone was able to encode such a behaviour. In order to model such properties a linear combination of several structural descriptors was used. Structural interpretation of such models is very difficult in most cases. Only recently, a modification of the variable connectivity index was introduced, which takes into account positive as well as possible *negative* contributions of atoms or bonds in structure-property-activity relationships (M. Pompe, Variable connectivity index as a tool for solving the 'anticonnectivity' problem, *Chem. Phys. Lett.,* 404(2005)296–299; COBISS.SI-ID 26572037, JCR IF: 2,438). Thus modified variable connectivity index of order zero was used for modelling the flame ionization detector (FID) response factors. Afterwards, the definition of the modified connectivity index of zero order was extended to higher order connectivity indices. These were introduced to account for the combination of positive and negative relative contributions of atoms and bonds in the construction of the QSPR models (M. Pompe, M. Randić: "Anticonnectivity": a challenge for structure-property-activity studies, *J. Chem. Inf. Mod.,* 46(2006)2–8; COBISS.SI-ID 27323141, JCR IF: 3,423). The coding capabilities of modified descriptors were presented in the modelling of the atmospheric reaction rate constants of selected organic compounds with OH radicals. The linear regression model, using a single structural descriptor, i.e., variable connectivity index of order one, produced root-mean-square error of 0.343 log units. Although the obtained calculation error was higher than in multiple linear regression models reported before, the new model offered important insight into the role of the individual structural components that influence the reactivity of organic compounds.

CHEMILUMINESCENCE – A TOOL FOR INVESTIGATING THE DEGRADATION OF CELLULOSE

Chemiluminescence has been in use in polymeric materials research for a number of years. Recently, it has found application in cellulose degradation research. The studies, which we coordinated within the framework of the 5th FP EU project Papylum, showed that in addition to temperature, chemiluminescence of celllulose critically depends on humidity as well. In order to study the related phenomena, we had to develop a new instrument, by which this parameter could be controlled. The results confirmed that water content has strong impacts on the rate of degradation of cellulose at temperatures below 100 °C, and we found several explanations. By experiments at elevated temperatures we found out that degradation proceeds at the maximum rate in an atmosphere containing 60–80% RH, whereas the rate decreases at lower and at higher temperatures. To study this phenomenon in more detail, we used dynamic chemoluminometric experiments in a humid atmosphere. This was only possible with the newly developed instrument. The experimental data have shown that superoxide anion could be a possible precursor of chemiluminescent species. The results were presented in a scientific paper (D. Kočar, M. Strlič, J. Kolar, J. Rychlý, L. Matisová-Rychlá, B. Pihlar, Chemiluminiscence from paper III: the effect of superoxide anion and water, *Polym. Degrad. Stab.*, 88(2005)407–414, COBISS.SI-ID 26572549, JCR IF: 1,749), and in a doctoral thesis (COBISS.SI-ID 28554757), which was granted the Samec Award (FCCT, 2007), and in several book chapters (COBISS.SI-ID: 219327232, 28510213). The achievements represent a very important contribution to understanding material degradation in objects of cultural heritage.

STABILITY OF HISTORICAL DOCUMENTS CONTAINING IRON GALL INK

Iron gall (tannic) inks have been used from the mediaeval times in Western cultures by many artists and represent the most important inks used at that time.. It is well known that iron and other metals contained in the inks, have a corrosive effect on paper, which leads to rapid degradation of the documents containing iron gall ink. We researched the causes of degradation within the framework of two EU 5th FW projects (InkCor and MIP) and described some of the most important parameters which influence ink stability in the scientific journal *Analytica Chimica Acta* (JCR IF: 2,894). The results indicate that the amount of ink and the concentration of acids mainly contribute to ink instability (J. Kolar, A. Štolfa, M. Strlič, M. Pompe, B. Pihlar, M. Budnar, J. Simčič, B. Reissland: Historical documents containing iron gall ink – properties affecting their condition, *Anal. Chim. Acta*, 555(2006)167–174; COBISS.SI-ID 19492391). Since it turned out that some inks were more corrosive than others, we were mainly interested in the explanation of this behaviour. We used a number of newly developed analytical methods, including PIXE (COBISS.SI-ID 19596071), as well as potentiometric determination of the pH of ink. By statistical analysis of data we were able to prove that corrosivity of ink is mostly influenced by the amount of ink applied, the pH of ink and paper grammature. Based on the data, mainly obtained from non-destructive methods, we were able to predict the stability of historical documents, which we also described in several chapters of the monographic publication (COBISS.SI-ID 28288773). The work represents an important contribution to the knowledge of degradation of historical documents.

HIGH PERFORMANCE METHOD FOR DETERMINATION OF PESTICIDES

Due to extensive use, pesticides and their degradation products represent severe health hazards. Therefore, a reliable determination in environmental samples and food are in focus of analytical science. In the publication which appeared in *Journal of Chromatography* A (The paper is ranked among 50 most cited papers in that journal in the period 2002–2007), we described GC-MS method for determining pesticides in fruits and vegetables. (D. Štajnbaher, L. Zupančič-Kralj, Multiresidue method for determination of 90 pesticides in fresh fruits and vegetables using solid-phase extraction and gas chromatography-mass spectrometry, *J. Chromatogr.* A, 1015 (2003)185–198; COBISS.SI-ID 25393925], JCR IF 2,922). The method is based on the pre-treatment of samples using solvent extraction of pesticides into acetone and combination of preconcentration/clean-up procedure using solid phase extraction (SPE) and ion exchange (IEX). After the optimization of the sample preparation step, chromatographic parameters, and MS detection, it was possible to simultaneously determine up to 90 pesticides with precision below 10% (RSD). The method was additionally improved by introducing a programmable temperature vaporizer (PTV) which enables the supply of larger sample volumes (10 µL) into the GC-MS system (D. Štajnbaher, L. Zupančič-Kralj, Optimisation of a programmable temperature vaporizer-based large volume injection for determination of pesticide residues in fruits and vegetables using gas chromatography-mass spectrometry, *J. Chromatogr.* A, 1190(2008)316–326; COBISS.SI-ID 29445381, JCR IF (2006): 3.554). By miniaturizing the step in sample preparation step using reverse phase extraction (RP-SPE) and by application of PTV module, it is possible to simultaneously identify and quantitatively determine 124 pesticides. Highly efficient method with low limit of quantification (0.01 mg/kg) can provide better and faster analysis and better control of food products, and can contribute to food safety which is among the important priorities in Slovenia and worldwide.

AGEING AND STABILISATION OF PAPER

The research oriented into degradation and ageing of cellulosic materials was part of the EU 5th FP project Papylum (EVK4-CT-2000-00038), coordinated by our group. In addition to many scientific publications in journals, we also published a monograph (*Ageing and stabilisation of paper*, Edited by M. Strlič and J. Kolar, National and University Library, Ljubljana, 2005, ISBN 961-6551-03-5, COBISS.SI-ID 219327232). It has been published in English and contains 211 pages of the latest information on cellulose degradation and processes governing paper ageing. Twelve chapters are divided into three sections: Methodology, Degradation and Stabilisation, which cover the most significant processes and methods used in paper degradation research. Eight chapters have been co-authored by programme group members and describe the achievements in the area of analytical characterisation of paper, thermo-oxidative degradation of paper and stabilisation strategies (COBISS.SI-ID: 26642693, 26642949, 26643205, 26643461, 26643717, 26643973, 26650373, 26650885). This monograph is a handbook, useful for researchers as well as for conservators and those concerned with conservation of paper-based cultural heritage. The engagement of researchers and the achievements in this research have qualified the co-workers of the laboratory and the programme group among the top internationally recognised experts. The knowledge acquired will be incorporated into university studies of the Faculty of Chemistry and Chemical Technology in the »Characterisation and Stability of Cultural Heritage Materials« course.

INTERNATIONAL SYMPOSIUM ON SEPARATION SCIENCES

In September 2006, the 12th International Symposium on Separation Sciences was organized by the Division for Analytical Chemistry of the Slovenian Chemical Society and Austrian Society for Analytical Chemistry (M. Strlič, W. Buchberger Editors, 12th International Symposium on Separation Sciences, Lipica, Slovenia, September 27th–29th, 2006. Book of abstracts: Lipica 2006. Ljubljana: Slovenian Chemical Society, 2006. 356 p., ISBN 961-90731-6-9, ISBN 978-961-90731-6-2, COBISS.SI-ID 228508416).

The symposium, chaired by Prof. Lucija Zupančič-Kralj, took place in Lipica, Slovenia, with 192 participants, approximately one third being from Slovenia. This event was partially financed by ARRS. The International Scientific Committee was composed of 15 respected and internationally recognized scientists. 153 scientific contributions were presented in the form of lectures and posters, and abstracts were published in the Book of abstracts which can be from the web. From Symposium contributions, 22 peer-reviewed papers have been published in a special issue of *Acta Chimica Slovenica* (COBISS.SI-ID 28517893). During symposium two workshops and an exhibition of analytical equipment were organized. Considering great interest in this event, it may be concluded that the main goal (transfer of knowledge into practice) has been achieved and that the organizational scheme (lectures, workshops, exhibition and posters) was appropriate and attractive both, from academic as well as users' point of view (there were 45 participants from industry). There were several presentations of programme group members at this symposium, which made an important contribution to the promotion of Slovenian science.

NEW PROCEDURES FOR STABILISATION OF HISTORIC DOCUMENTS

Within the framework of the 5. FP project InkCor (EVK4-CT-2001-00049), coordinated by J. Kolar, and by M. Strlič at the level of UL, we investigated the corrosiveness of iron gall inks

and developed methods for stabilisation of documents containing such inks. Our involvement in this project was very successful, resulting in numerous scientific papers, and publication of a scientific monograph (»*Iron gall inks: on manufacture, characterisation, degradation and stabilisation*«, National and University Library, Ljubljana, 2006 (ISBN 961-6551-19-1, ISBN 978-961-6551-19-9, COBISS.SI-ID 230700544). The monograph describes various aspects of historical iron galls inks, from preparation, to model studies and degradation studies. Within this project we also developed a new technological procedure for material stabilisation using antioxidants, which we described in a patent application (COBISS.SI-ID 26939909). The efficiency of the proposed treatment was tested on a variety of inks and materials. This new product has been commercialised by the German company Zentrum für Bucherhaltung GmbH. In the book, its use is described and evaluated. Several chapters have been co-authored by programme group members (COBISS.SI-ID: 28288773, 28289285, 28289797, 28290309, 28290565). Our achievements are particularly important for long-term stabilisation and conservation of paper-based cultural heritage and strongly contribute to the promotion of Slovenian science.

MICROELECTRODE FOR pH DETERMINATION OF PAPER

Glass electrodes are most often used for pH determination. However, such analyses lead to sample destruction or damage paper. It is well known that pH in macromolecular environment is one of the most important parameters which defines paper lifetime. However, most of the pH determination procedures used nowadays are not suitable, including miniaturised pH glass electrode, due to mechanical instability. Therefore, we developed a new, robust electrode made of glassy carbon, onto which a thin layer of polyaniline was electrodeposited (M. Strlič, B. Pihlar, L. Mauko, J. Kolar, S. B. Hočevar, B. Ogorevc: A new electrode for micro-determination of paper pH, *Restaurator,* 26(2005)159–171; COBISS.SI-ID 3342874). The electrode was tested on a variety of real papers and the accuracy of results was compared with those obtained from standard procedures. Since the electrode is especially suitable for determining the pH of paper in a non- or micro-destructive manner, we also manufactured the electrode holder (for both the indicator and the reference Ag/AgCl electrodes), which enables straightforward calibration and measurement of pH of paper and induces minimal damage to the original material. We also researched the influence of interferences and the calibration. With electrode prototype we could determine the pH directly on the original document using minimal amount of water (1–2 µl). The procedure was tested on numerous real samples and we obtained extremely positive feedback from the potential end-users. Technical prototype was developed on the basis of the laboratory prototype and was partly carried out within the project Eureka 3843. In the future, we are planning to further develop the prototype and market the product with the spin-off company Morana RTD.

VOLATILE ORGANIC COMPOUNDS IN THE AIR

An overview of the several years's research on the determination of volatile organic compounds (VOCs) in the air was presented in an invited lecture. Gas chromatography (GC) or high performance liquid chromatography (HPLC) coupled with mass spectrometry (MS), or other detectors are two most commonly used techniques for determining VOCs or their atmospheric oxidation products. Since we are dealing with non-target analysis, we are facing two main problems, i.e. accurate identification and quantification of individual VOCs. The identification is performed by using MS detector in combination with numerical prediction of retention times. The other problem is quantification in the trace level (ppb down to ppt). To

overcome this problem a very efficient pre-concentration step should be used, i.e., pre-concentration on adsorption tubes, followed by thermal desorption. Several different analytical techniques were presented for the determination of anthropogenic and biogenic VOCs and their oxidation products. The results of a long-term research were presented as an invited lecture at the meeting of the Slovenian Chemical Society (M. Pompe, M.Veber, Determination of volatile organic compounds in the air, P. Glavič (ur.), D. Brodnjak Vončina (ur.), Slovenski kemijski dnevi 2005, Maribor, 2005; (COBISS.SI-ID 27020805) and represent an original scientific contribution to environmental protection.

In addition to the results mentioned above, we need to emphasise the following achievements:

a) A quantitative structure-property research study was performed to predict thermodynamic values, i.e., ΔS^o and ΔH^o for the separation processes using gas chromatography (COBISS.SI-ID 25800197). The procedure allows for accurate identification of organic compounds in homological series of n-alkanes, 1-alkenes and 2-alkenes. Variable connectivity indices of different orders were used for the modelling of atmospheric reaction rate constants (COBISS.SI-ID 26342917, COBISS.SI-ID 29915397) and pK_a values of some halogenated organic acids (COBISS.SI-ID 28928005). Simple mathematical representations of the chemical structure were applied in modelling the properties of benzenoid compounds as well (COBISS.SI-ID 28508165), some of which are cancerogenic. Furthermore, it was shown that π-electron signatures can be used for the classification of benzenoid compounds (COBISS.SI ID 29447429, COBISS.SI-ID 29976325).

The influence of matrix components (HNO_3, MeOH) on the determination of phosphorus by elemental mass spectrometry was studied (COBISS.SI-ID 3386650) and two low-cost analytical instruments – a gas chromatograph (COBISS.SI-ID 1246044]) and spectrophotometric microtitrator (COBISS.SI-ID 25549829, 28579077) intended for educational purposes were developed. Experimental conditions for a simultaneous ion chromatographic determination of major and minor ions in seawater and derived saline solutions were optimised, and the determined ionic composition of water samples was related to other water quality parameters (COBISS.SI-ID 29873157). Liquid chromatographic (HPLC) and micellar electrokinetic chromatographic (MEKC) methods for the determination of non-volatile pesticides (atrazine) and its decomposition products have been developed and applied to the studies of interactions between humic substances and some mineral components in the environment (COBISS.SI-ID 26061829).

In collaboration with the industry LEK d.d. a fast chromatographic method for the separation of pravastatine, mevastatine and 6-epi pravastatine in fermentation production media has been developed (COBISS.SI-ID 84418). Separation in this complex medium was achieved in one minute. This method enables efficient control of biosynthesis in pharmaceutical production. In collaboration with the company Krka d.d., parameters for the release of diclofenac sodium from lipophilic matrix tablets (COBISS.SI-ID 26133765) were studied and two level-six-factorial experimental design was applied to optimize the conditions for drug release studies (COBISS.SI-ID 1438577). In collaboration with the company BIA we investigated the possibilities for the application of monolithic chromatographic columns for fast isolation and partial fractionation of proteins (COBISS.SI-ID 1298268). With the National Institute of Chemistry the computer programme for modelling of anion separation in IC was developed (COBISS.SI-ID 3858970).

b) The parameters which influence depolymerisation of cellulose and paper have been studied, as well as corrosion properties of historical iron gall ink and its influence on the degradation of paper. Corrosion studies were also performed on other materials (e.g. Co and Cu-Zn alloys).

The properties of cellulose fibres (crystallinity, morphology and size) on paper chemiluminescence were investigated (COBISS.SI-ID 26156037). Using ^{13}C-1 labelled glucose oxidation of cellulose end-groups and the phenomena of self-absorption of light during chemiluminescence of paper was studied and quantitatively explained (COBISS.SI-ID 29192453). Another study was on photooxydation of cellulose (COBISS.SI-ID 26628357) and catalytic effect of some halide ions and metals on the role of Fenton processes in oxidative degradation of cellulose. (COBISS.SI-ID 27068677, 28858373). With the use of NIR spectroscopy and chemometrics, mechanical properties of historical papers were investigated and a new instrument developed (COBISS.SI-ID 29804549). Corrosion properties of iron in gall ink have been described in several papers and new analytical methodology for the evaluation of deteriorated historical documents is proposed (COBISS.SI-ID 214488576). XANES spectroscopy was employed for the determination of Fe (II) / Fe (III) ratio in historical gall inks that significantly influence their corrosion properties (COBISS.SI-ID 665339). It has been proved that proper selection of reference compounds is very important for this technique and that it strongly influences the reliability of analytical results. They should have the same symmetry with neighbouring atoms and same local structure compared to original samples.

In order to find an efficient inhibitor that could be used also for the application and preservation of historical documents in non-aqueous media two myo-inositol phosphates (COBISS.SI-ID 27520261) were synthesized, which indicate similar inhibitory properties as pyhtic acid. Using ^{31}P NMR and X-ray techniques we investigated the interactions and structure of Fe(III) inositol hexaphosphates (COBISS.SI-ID 3617562). The processes for the stabilization of iron gall ink containing documents waere investigated (COBISS.SI-ID 27066373) and an improved procedure, based on the treatment with magnesium phytate, was proposed (COBISS.SI-ID 29238533) We also investigated the possibilities for controlled cleaning of paper and documents using laser (COBISS.SI-ID 26905605).

In an extensive study and critical evaluation of the existing procedures for pH measurements of paper (COBISS.SI-ID 26114309), theoretical, as well as experimental parameters that influence accuracy of potentiometric and colorimetric measurements were considered and evaluated. Based on these findings a robust glassy carbon microelectrode modified with polyaniline was developed (COBISS.SI-ID 3342874), which allowed for local measurement of pH in documents with minor interaction with the sample. With the analysis of volatile organic compounds (VOC) emitted from paper it was proven that by the use of advanced instrumentation and proper analytical approach we could achieve a completely non destructive pH determination of historical documents (COBISS.SI-ID 29134853). This method is based on the GC-MS measurements of furfural emitted from paper which correlate well with the pH of the paper. The research on metallic materials was oriented towards stability studies of Co alloys in physiological media (COBISS.SI-ID 17668313, 18268711) and processes that influence the corrosion properties of Cu-Zn alloys (COBISS.SI-ID 18793255, 19217959).

c) Within the research programme related to the pollution of the environment, food and investigation of biological systems, the use of microwave extraction of some selected pesticides from soil samples was investigated (COBISS.SI-ID 621526) as well as kinetics of photochemical transformation of atrazine and its degradation products in the environment (COBISS.SI-ID 26342405). For studies on the distribution and sorption of selected contaminants (PCBs, chlorosubstituted insecticides, triazine and amide herbicides) on humic acids, soil and mineral constituents, solid phase micro-extraction was applied (COBISS.SI-ID 28423173). Size exclusion chromatography and ICP-MS were applied for sorption studies of some metal ions on humic substances (COBISS.SI-ID 28522245) and sensitive method for selenium determination in plant material based on the application of HPLC-UV-Hg-AFS was elaborated (COBISS.SI-ID 19685671).

A new method for determining ochratoxin A in wine based on on-line extraction and HPLC separation in combination with fluorimetric and MS detection was developed. The method was applied in photostability studies of ochratoxin A at daylight (COBISS.SI-ID 27677957). An extraction procedure for determining the constituents of must and wine aroma based on solid phase micro-extraction (DVB/CAR/PDMS fibres) and GC-MS and HPLC-MS identification/ quantification of specific compounds was developed(COBISS.SI-ID 4982649, 5326969]). Determination of free amino acids (AA) in musts and young wines using pre-column derivatization with 3-MPA/OPA for primary AA and FMOC-Cl for secondary AA was studied. As sugar content considerably differs in samples the influence of sugars on derivatization was investigated using two internal standards: (i) primary AA norvaline and (ii) secondary AA sarcosine, in real samples and in model fructose and glucose solutions. A strong matrix effect was observed, especially when concentrations of sugars exceeded 50 g/L (COBISS.SI-ID 29802245).

Interactions of quinolone ciprofloxacin with Cu (I) and Cu (II) were studied (COBISS.SI-ID 1668977) and the isolation of lysophosphatidic acid (LPA) from human plasma as a potential biomarker for ovarian tumor cancer was developed (COBISS.SI-ID 2189937). The HPLC-MS/MS analytical method was applied for determining LPA in the serum of patients with different ovarian tumor (COBISS.SI-ID 23159001). It was ascertained that LPA content in serum correlates with tumor presence, however, the method does not provide a reliable differentiation between benign and malignant tumors.

Furocoumarins naturally occur in different plants (mainly Citrus species) and exert several physiological effects, which imply the need to control their concentration in the products intended for human use. We developed a LC-MS/MS method combined with solid-phase extraction (SPE) for bergapten and bergamottin in different samples of beverages and cosmetics. Due to pronounced matrix effects, standard addition method for quantification yielded the most reliable results (COBISS.SI-ID 29682437).

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, ki se je v letu 2008 zaključil, 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 letih 2004–2008 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 nanožičk in kompozitov iz nanožičk. V tem sklopu smo študirali sintezo in lastnosti, 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 smo ga v letu 2008 obnovili, pri tem nam je UL FKKT nesebično pomagala. 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 2008 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. V letih 2009–2013 bomo nadaljevali z raziskavami v tej programski skupini.

ZNANSTVENI DOSEŽKI 2004–2008

Omeniti velja zlasti naslednje dosežke:

Korelacije struktur v raztopinah in v trdnem stanju

1H in 19F NMR spektri raztopin $(C_5Me_4R)TiF_3$ (R = H, Me, Et) so pokazali na prisotnost sedmih molekul, od monomere do tetramer. Termodinamski in kinetični parametri, izmerjeni za pretvorbe med temi molekulami, so nam omogočili predlagati mehanizme teh procesov. Ravnotežje med monomero in dimero $(C_5Me_4R)TiF_3$ kaže na analogno ravnotežje v raztopinah spojin s Ti-F vezjo. To ravnotežje tudi omogoča pojasnitev obnašanja homogenih fluorotitanovih katalizatorjev. Pri teh katalizatorjih so opazili enantioselektivno ojačitev. Ta učinek je lahko zaradi katalitično aktivnih monomer ali dimer. Naše raziskave kažejo, da so aktivne

katalitične oblike pri fluorotitanovih katalizatorjih momomere. Ti rezultati bodo olajšali načrtovanje novih katalizatorjev tega obetavnega tipa.

– PERDIH, Franc, PEVEC, Andrej, PETRIČEK, Saša, PETRIČ, Andrej, LAH, Nina, KOGEJ, Ksenija, DEMŠAR, Alojz. The solution structures and dynamics and the solid-state structures of substituted cyclopentadienyltitanium(IV) trifluorides. Inorg. chem., 2006, vol. 45, no. 19, str. 7915–7921.

Bakrova kompleksna spojina učinkovito cepi DNK

V članku je objavljena nova bakrova kompleksna spojina, ki učinkovito hidrolitično cepi DNK. Gre za kvadratno planaren kompleks [Cu(Hpyrimol)Cl], ki je dobro topen v vodi. Podani so tudi rezultati citotoksičnosti za določene rakaste celice. Bakrov kompleks uspešno cepi X174 in izkazuje citotoksičnost proti L1210 levkemiji in A2780 raku pri človeku. Vrednosti so primerljive ali celo boljše od onih za cisplatino.

– MAHESWARI, Palanisamy Uma, ROY, Sudeshna, DULK, Hans den, BARENDS, Sharief, WEZEL, Gilles van, KOZLEVČAR, Bojan, GAMEZ, Patrick, REEDIJK, Jan. The square-planar cytotoxic [Cu[sup]II(pyrimol)Cl] complex acts as an efficient DNA cleaver without reductant. J. Am. Chem. Soc., 2006, vol. 128, no. 3, str. 710–711.

Nanožičke

Z rentgensko praškovno difrakcijo smo rešili in analizirali strukturo $Mo_6S_{9-x}I_x$ nano-žičk, ki kažejo nekatere zelo zanimive lastnosti (na primer izjemna natezna trdnost vzdolž vlaken) in so bile pripravljene v drugi programski skupini. Ker gre za nov material je bil strukturni tip neznan, zaradi majhnih dimenzij in morforlogije (vlakna) je bila določitev strukture izredno zahtevna, ko pa smo uspeli dobiti strukturni model, se je le-ta izkazal kot pravilen tudi po preverjanju z drugimi metodami (ki ne morejo rešiti strukture – dobiti začetnega strukturnega modela – lahko pa preverijo ustreznost različnih modelov). Tudi zato ima članek že v tretjem letu po objavi 17 čistih citatov.

– MEDEN, Anton, KODRE, Alojz, PADEŽNIK GOMILŠEK, Jana, ARČON, Iztok, VILFAN, Igor, VRBANIĆ, Daniel, MRZEL, Aleš, MIHAILOVIĆ, Dragan. Atomic and electronic structure of $Mo_6\ S_{9-x}\ I_x$ nanowires. Nanotechnology (Bristol), 2005, 16, str. 1578–1583.
– VRBANIĆ, Daniel, REMŠKAR, Maja, JESIH, Adolf, MRZEL, Aleš, UMEK, Polona, PONIKVAR, Maja, JANČAR, Boštjan, MEDEN, Anton, NOVOSEL, Barbara, PEJOVNIK, Stane, VENTURINI, Peter, COLEMAN, Jonathan N., MIHAILOVIĆ, Dragan. Air-stable monodispersed $Mo_6S_3I_6$ nanowires. Nanotechnology (Bristol), 2004, vol. 15, str. 635–638.

Katodni material za litijeve baterije

V sodelovanju z drugo programsko skupino smo v naši programski skupini z rentgensko praškovno difrakcijo določili strukturo novega materiala za katodni material litijevih akumulatorjev (izostrukturna Li_2MSiO_4, M=Fe,Mn). Rešena struktura je omogočila razumevanje in načrtno spreminjanje transportnih lastnosti materiala (potovanje litijevih ionov skozi kanale oktaedričnih praznin v heksagonalnem najgostejšem skladu kisika) in pristop z računskimi metodami, ki potrebujejo začetni strukturni model.

– DOMINKO, Robert, BELE, Marjan, GABERŠČEK, Miran, REMŠKAR, Maja, MEDEN, Anton, REMŠKAR, Maja, JAMNIK, Janko. Structure and electrochemical performance of Li_2MnSiO_4 and Li_2FeSiO_4 as potential Li-battery cathode materials. Electrochem. commun., 2006, vol. 8, no. 2, str. 217–222).

In vitro raziskave z vanadijevimi koordinacijskimi spojinami

V tej sistematični študiji različnih vanadijevih(IV in V) spojin smo preučevali njihovo sposobnost pri stimuliranju vnosa glukoze v celice (insulinsko mimetična lastnost). Korelacije med naravo liganda in aktivnostjo ni bilo moč jasno odkriti. Kot ligand smo uporabili tudi kinolonski ligand. To interdisciplinarno zasnovano delo je bilo v zadnjem času visoko citirano.

– REHDER, Dieter, PESSOA, João Costa, GERALDES, Carlos F. G. C., CASTRO, M. Margarida C. A., KABANOS, Themistoklis, KISS, Tamás, MEIER, Beate, MICERA, Giovanni, PETTERSSON, Large, RANGEL, Maria, SOLIFOGLOU, Athanasios, TUREL, Iztok, WANG, Dongren. In vitro study of the insulin-mimetic behaviour of vanadium(IV, V) coordination compounds. JBIC, J. biol. inorg. chem. (Print), 2002, vol. 7, no. 4/5, str. 384–396.

DRUGI RELEVANTNI DOSEŽKI

1. IZBOLJŠANJE OBSTOJEČEGA TEHNOLOŠKEGA PROCESA OZ. TEHNOLOGIJE

Skupina raziskovalcev programske skupine sodeluje z Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika (Pogodba št. KPIOT-2/2007) pri izboljševanju praktične sinteze in proizvodnje železovega kompleksa z EDTA, ki ga v Unichemu pripravljajo za prodajo.

2. EUROPEAN UNIVERSITY ASSOCIATION – EVALUATION EXPERT POOL

I. Leban je član ekspertnega poola za institucionalno evalvacijo evropskih univerz. V letu 2007 je bil član dveh evalvacijskih komisij:

– Kralj, A., Stanković, F., Leban, I., Bašić, F., Koprivica, S.: Izvještaj o spoljašnjoj evaluaciji u postupku reakreditacije Univerziteta Crne gore i njegovih studijskih programa, Podgorica : Savjet za visoko obrazovanje Crne gore, 2007, 166 str.
– Lamicq, H., Nazare, M.H., Leban, I., Kladis, D.: Ege University : EUA review report, Brussels : European University Association, 2007, 41 str.

3. COST D20-0006/01 METAL ION COMPLEXES WITH ANTIBACTERIAL QUINOLONES AND ANTIVIRAL NUCLEOTIDE ANALOGUES

Koordinator in odgovorni nosilec: I. Turel.

Po sodelovanju v eni od skupin projekta COST D8 je v naslednjem obdobju (2001–2006) postal koordinator ene od skupin v okviru COST D 20. Naša delovna skupina je vključevala 7 laboratorijev iz šestih evropskih držav. Bil je eden mlajših koordinatorjev pa tudi edini koordinator iz Slovenije v tem sklopu.

4. ZNANSTVENI PROGRAMSKI ODBOR EPDIC 10

Član programske skupine A. Meden je član Evropskega sveta za praškovno difrakcijo in je sodeloval v znanstvenem programskem svetu pri organizaciji 10. evropske konference o praškovni difrakciji (EPDIC 10, Geneva, Switzerland, September 2006). Skupaj A. Kernom iz Brukerja AXS je organiziral enega od mikrosimpozijev na tej konferenci (Določanje strukture iz enega praškovnega difraktograma).

5. ORGANIZACIJA IN PREDSEDOVANJE NA SLOVENSKO-HRVAŠKIH KRISTALOGRAFSKIH SREČANJIH

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

2004 13th Slovenian-Croatian Crystrallographic Meeting, Bovec.
2005 14th Croatian-Slovenian Crystallographic Meeting, Vrsar
2006 15th Slovenian-Croatian Crystallographica Meeting, Jezersko
2007 16th Croatian-Slovenian Crystallographic Meeting, Petrčane-Zadar
2008 17th Slovenian-Croatian Crystallographic Meeting, Ptuj

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

6. MEDNARODNO SODELOVANJE

- COST D20-0006: Metal Ion Complexes with Antibacterial Quinolones and Nucleotide Analogues (I.Turel)
- Bilateralno sodelovanje s Srbijo – 2005–2006: Sinteza in strukture kompleksov prehodnih kovin (I. Leban)
- Bilateralno sodelovanje s Češko 2006–2007: Organoaluminijtitanovi fluoridi (A. Demšar)
- Bilateralno sodelovanje z Avstrijo 2007–2008: Koordinacijski polimeri – od načrtovanja zgradbe do uporabnih materialov (I.Leban)
- 6. okvirni program: BioCellus – Biomass Fuel Cell Utility System (Uporaba biomase za gorivne celice) No. 502759 (J. Maček)
- Bilateralno sodelovanje s Hrvaško 2007–2008: Encimska kataliza – modelni sistemi: prenos protona v vodikovih vezeh z nizko energijsko bariero (A. Meden)
- Bilateralno sodelovanje s Srbijo 2008–2009: Struktura in mikrostruktura oksidnih nanomaterialov (A. Meden)

7. DRUGO SODELOVANJE

- Pogodba KPIOT-2/2007 z Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika (J. Golob, B. Kozlevčar, I. Leban)
- Sodelovanje s Salonitom, Anhovo (A. Meden, J. Maček)
- Sodelovanje s Krko, Novo mesto (A. Meden)

8. PROMOCIJA ZNANOSTI

Noč znanstvenic in znanstvenikov 2006, 2007, 2008 (A. Knez, M. Francetič, I. Leban)
http://abra.fkkt.uni-lj.si/fn01leban/rn2006/
http://abra.fkkt.uni-lj.si/fn01leban/rn2007/
http://abra.fkkt.uni-lj.si/fn01leban/rn2008/

KOMENTAR ZA ZAKLJUČEK

Kot vsaka temeljna raziskava tudi naša raziskava vpliva na družbeni in kulturni razvoj Slovenije. Tak tip raziskav ni pomemben samo za razvoj osnovnih znanj, ampak omogoča tudi vključevanje dodiplomskih in podiplomskih študentov v neposredno raziskovalno delo in s tem stalen prenos znanja in izkušenj na mlajše raziskovalce. Znanja, ki si jih bodo študentje pridobili pri delu na teh raziskavah, bodo uporabna tudi za njihovo kasnejše poklicno delovanje. Raziskave so zasnovane kot temeljne, vendar se dobljena znanja lahko tudi koristno uporabijo. Rezultati raziskav so lahko torej dobra osnova za nadaljnje razvojno in raziskovalno delo, ki bi omogočilo uporabo sintetiziranih spojin in materialov v različne namene. Vnaprej napovedovati, kaj bo koristno in kaj ne, pa je zelo vprašljivo. Raziskave so neposredno vezane na predmetnik podiplomskega študija (smeri: kemija, kemijska tehnologija, biokemija) na UL FKKT. To so npr. predmeti: Koordinacijska kemija, Rentgenska strukturna analiza, Aplikativna kristalografija, Bioanorganska kemija, Organokovinska kemija in drugi. Temeljne raziskave prispevajo: – k narodovi kulturi; – lahko omogočijo odkritja, ki se kasneje izkažejo za zelo koristna; – pripomorejo k razvoju gospodarstva; – in so sestavni del vzgojno-izobraževalnega sistema. Vredno bi bilo omeniti tudi težave, s katerimi se soočamo. Politika visokošolskega izobraževanja in raziskovanja gre v smer »starega modela« – izobraževanje naj bi potekalo na univerzah in visokih šolah, kvalitetno raziskovalno delo (tudi primerno financirano) pa naj bi potekalo na raziskovalnih inštitutih. Tudi vpeljava »Bolonjske reforme« poteka v tej smeri, za univerze naj bi bile rezervirane 1. in 2. bolonjska – strokovna – stopnja, doktorske šole (3. stopnja) pa naj bi se opravljale na inštitutih. Zato se dogaja, da število doktoratov z univerzitetnimi mentorji upada in se večina doktorjev zaposluje na inštitutih. Nihče se ne zaveda dejstva, da morata biti raziskovanje in izobraževanje neločljivo povezana. Nedavni primer združitve med Univerzo v Karlsruheju in Forschungszentrum Karlsruhe nam dokazuje, kako lahko nastane elitna univerzitetna inštitucija z dovolj veliko kritično maso. Prav zato bi morali narediti analizo stanja in rezultatov v našem visokem šolstvu in raziskovalnem prostoru (npr. cost/benefit, tudi s tujimi strokovnjaki) in sprejeti ustrezne koristne spremembe oz. priporočila. To bomo morali izvajati tudi zaradi članstva v OECD.

Zelo primerno bi bilo imeti tudi javno dostopno bazo vseh relevantnih podatkov v zvezi z izobraževanjem in raziskovanjem. Nenazadnje moramo te podatke redno posredovati EUROSTAT-u.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

The main objective of the research programme from 2004–2008, which is expiring, 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 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 on powder samples as well. For this kind of research we employed the methods and tools for X-ray diffraction and some research time was 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 in searching and explaining other properties correlated with the structure (mechanical, optical, thermal, stability, etc.). The correlation between the structural and biological properties is also of fundamental importance for understanding nature. In 2007 we explicitly focused on collaboration with industry. This part of research was connected with the work of the Chair of Inorganic Chemistry.

During 2004–2008 the research activities of the Chair of Inorganic Chemical Technology and Materials was directed towards studying complex reaction systems and preparation of products with designed properties and characteristics.

Research of electrocatalytic materials for high temperature systems of fuel cells was 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 have 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 as the electro-catalyst 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 electro-conductivity of the material are directly determined by the initial processes and conditions of sintering of the composite. Part of the research was also directed towards homogenous co-precipitation 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 nanowires and composites of nanowires. Tribological performances, electrical conductivity and nanomechanical properties of nanowires were studied.

RESEARCH TOPICS

Our research is divided into two parts: fundamental and applied research. Thus, we can say that the Chair of Inorganic Chemistry has a strong and modern synthetic research team (**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. 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. The research will continue in the period 2009–2013.

SCIENTIFIC ACHIEVEMENTS

CORRELATION BETWEEN THE SOLUTION AND SOLID-STATE STRUCTURES

The 1H and 19F NMR spectra revealed equilibria of seven different species in the solutions of $(C_5Me_4R)TiF_3$ (R=H, Me, Et) ranging from monomer to tetramer. The thermodynamics and kinetics of dimerization and dissociation involving monomers and dimers allowed for the prediction of mechanisms of these processes. It is obvious that the relative stabilities of dimers and monomers of species with a Ti-F bond depend on other groups bonded to titanium. However, the equilibrium of monomer and dimer of $(C_5Me_4R)TiF_3$ suggests that both, monomer and Ti-(μ-F)2-Ti dimer can be expected in compounds with a Ti-F bond. This equilibrium could help understand the behavior of homogeneous fluorotitanium catalysts and suggests catalysis with more-active monomers, as already proposed. The catalytic system with partially resolved chiral ligands on titanium could achieve chiral amplification on the basis of the catalytically active monomers. The additional requirements for chiral amplification in such a system are different stabilities of the homochiral and heterochiral dimer.

– PERDIH, Franc, PEVEC, Andrej, PETRIČEK, Saša, PETRIČ, Andrej, LAH, Nina, KOGEJ, Ksenija, DEMŠAR, Alojz. The solution structures and dynamics and the solid-state structures of substituted cyclopentadienyltitanium(IV) trifluorides. Inorg. chem., 2006, vol. 45, no. 19, str. 7915–7921.

SQUARE-PLANAR COPPER COMPLEX ACTS AS AN EFFICIENT DNA CLEAVER

The novel DNA cleavage properties of highly water-soluble, square-planar [Cu(Hpyrimol)Cl] complex, together with the results of cytotoxicities toward selected cancer cell lines is reported. The copper complex cleaves X174 supercoiled DNA efficiently and shows high cytotoxicities toward L1210 murine leukemia and A2780 human ovarian carcinoma cancer cell lines that are sensitive and resistant to cisplatin. The IC50 values obtained for the copper complex in sensitive cell lines are in the range of cisplatin.

– MAHESWARI, Palanisamy Uma, ROY, Sudeshna, DULK, Hans den, BARENDS, Sharief, WEZEL, Gilles van, KOZLEVČAR, Bojan, GAMEZ, Patrick, REEDIJK, Jan. The square-planar cytotoxic [Cu[sup]II(pyrimol)Cl] complex acts as an efficient DNA cleaver without reductant. J. Am. Chem. Soc., 2006, Vol. 128, No. 3, pp. 710–711.

NANOWIRES

X-ray powder diffraction was used to solve and analyze the structure of $Mo_6S_{9-x}I_x$ nano-wires which exhibit some very interesting properties (extraordinary tensile strength along the length of fibers, for example). The wires were synthesized in another research programme group. As the material was new, the structure type was unknown. Due to small dimensions and morphology (fibers), the structure determination was very difficult. However, when the structure model was determined it was proven correct after checking with other methods that are not capable to solve the structure, but can assess the feasibility of different models. This is one of the reasons that the article has been cited 17 times after the third year of its publication.

– MEDEN, Anton, KODRE, Alojz, PADEŽNIK GOMILŠEK, Jana, ARČON, Iztok, VILFAN, Igor, VRBANIĆ, Daniel, MRZEL, Aleš, MIHAILOVIĆ, Dragan. Atomic and electronic structure of $Mo_6 S_{9-x}I_x$ nanowires. Nanotechnology (Bristol), 2005, 16, pp. 1578–1583.
– VRBANIĆ, Daniel, REMŠKAR, Maja, JESIH, Adolf, MRZEL, Aleš, UMEK, Polona, PONIKVAR, Maja, JANČAR, Boštjan, MEDEN, Anton, NOVOSEL, Barbara, PEJOVNIK,

Stane, VENTURINI, Peter, COLEMAN, Jonathan N., MIHAILOVIĆ, Dragan. Air-stable monodispersed $Mo_6S_3I_6$ nanowires. Nanotechnology (Bristol), 2004, Vol. 15, pp. 635–638.

POTENTIAL LI-BATTERY CATHODE MATERIAL

Collaboration with another programme group resulted in structure determination of a novel material for cathodes of lithium accumulators (isostructural Li_2MSiO_4, M=Fe, Mn) using powder diffraction, performed by our group. Thus solved material structure helped to understand and target the change of transport properties of the material (travelling of lithium ions along channels of the octahedral interstices in the hexagonal closest packing of oxygen). After the structural model had been determined, the computing methods were applied.

– DOMINKO, Robert, BELE, Marjan, GABERŠČEK, Miran, REMŠKAR, Maja, MEDEN, Anton, REMŠKAR, Maja, JAMNIK, Janko. Structure and electrochemical performance of Li_2MnSiO_4 and Li_2FeSiO_4 as potential Li-battery cathode materials. Electrochem. commun., 2006, Vol. 8, No. 2, pp. 217–222.

IN VITRO STUDY OF THE INSULIN-MIMETIC BEHAVIOUR OF VANADIUM(IV, V) COMPOUNDS

In this systematic study of various vanadium (IV and V) compounds and their ability to stimulate glucose uptake by cells (insulin mimetic properties) were studied. No striking correlation between the nature of the ligand systems and the insulin-mimetic potency was found. Antibacterial quinolone was also used as a ligand. This interdisciplinary work has been recently highly cited.

– REHDER, Dieter, PESSOA, João Costa, GERALDES, Carlos F. G. C., CASTRO, M. Margarida C. A., KABANOS, Themistoklis, KISS, Tamás, MEIER, Beate, MICERA, Giovanni, PETTERSSON, Large, RANGEL, Maria, SOLIFOGLOU, Athanasios, TUREL, Iztok, WANG, Dongren. In vitro study of the insulin-mimetic behaviour of vanadium(IV, V) coordination compounds. JBIC, J. biol. inorg. chem. (Print), 2002, Vol. 7, No. 4/5, pp. 384–396.

OTHER RELEVANT ACHIEVEMENTS

1. IMPROVEMENT OF THE TECHNOLOGICAL PROCESS

Collaboration exists with the company Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika (Contract No. KPIOT-2/2007). The purpose is to improve the synthesis and the production of iron complex compound with EDTA. The product is intended for market production.

2. EUROPEAN UNIVERSITY ASSOCIATION- EVALUATION EXPERT POOL

I.Leban is a member of the expert pool of the European University Association which performs institutional university evaluation. In 2007 he was a member of two expert groups. Two reports are available:

– Kralj, A., Stanković, F., Leban, I., Bašić, F., Koprivica, S.: Izvještaj o spoljašnjoj evaluaciji u postupku reakreditacije Univerziteta Crne gore i njegovih studijskih programa, Podgorica : Savjet za visoko obrazovanje Crne gore, 2007, 166 p.
– Lamicq, H., Nazare, M.H., Leban, I., Kladis, D.: Ege University-Izmir, Turkey : EUA review report, Brussels : European University Association, 2007, 41 p.

3. COST D20-0006/01 METAL ION COMPLEXES WITH ANTIBACTERIAL QUINOLONES AND ANTIVIRAL NUCLEOTIDE ANALOGUES

Coordinator and principle investigator: I. Turel.

After participating in working group of COST D8 action programme, he was coordinating a working group within COST D 20 programme in the period 2001–2006. The group consisted of seven laboratories from sic European countries. I. Turel is one of the youngest coordinators and also the only coordinator from Slovenia within this action programme.

4. SCIENTIFIC PROGRAMME MEMBER OF THE 10TH EPDIC

Mr. A. Meden is a member of the European Powder Diffraction Conference Committee and acted as a scientific programme member of the 10th EPDIC in Geneva, Switzerland, September 2006. During this conference he organized, together with A. Kern from Bruker AXS, a microsymposium on Structure determination from a single powder diffraction pattern

5. ORGANIZATION AND CHAIRMANSHIP OF SLOVENIAN-CROATIAN CRYSTALLOGRAPHIC MEETINGS

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

2004 13th Slovenian-Croatian Crystrallographic Meeting, Bovec.
2005 14th Croatian-Slovenian Crystallographic Meeting, Vrsar
2006 15th Slovenian-Croatian Crystallographica Meeting, Jezersko
2007 16th Croatian-Slovenian Crystallographic Meeting, Petrčane-Zadar
2008 17th Slovenian-Croatian Crystallographic Meeting, Ptuj

There are on the average between 60 and 80 participants at each meeting.

6. INTERNATIONAL COOPERATION

- COST D20-0006: Metal Ion Complexes with Antibacterial Quinolones and Nucleotide Analogues (I.Turel)
- Bilateral Cooperation with Serbia – 2005–2006: Synthesis and Structure of Transition Metal Complexes (I.Leban)
- Bilateral Cooperation with Czhech Republic 2006–2007: Organoaluminumtitanium Fluorides (A. Demšar)
- Bilateral Cooperation with Austria 2007–2008: Coordination Polymers – Crystal Engineering (I.Leban)
- FP6: BioCellus – Biomass Fuel Cell Utility System (J. Maček)
- Bilateral Cooperatin with Croatia 2007–2008: Enzyme Catalysis – Model Systems: Proton Transfer in Low Barrier Hydrogen Bonds (A. Meden)
- Bilateral Cooperation with Serbia 2008–2009: Structure and Microstructure of Oxide Nanomaterials (A. Meden)

7. OTHER COOPERATION

- Contract KPIOT-2/2007 with the Unichem d.o.o., Sinja Gorica 2, 1360 Vrhnika (J. Golob, B. Kozlevčar, I. Leban)
- Collaboration with Salonit, Anhovo (J. Maček, A. Meden)
- Collaboration with Krka, Novo mesto (A. Meden)

8. POPULARISATION OF SCIENCE

Researchers' Night, 2006, 2007, 2008 (A. Knez, M. Francetič, I. Leban)
http://abra.fkkt.uni-lj.si/fn01leban/rn2006/
http://abra.fkkt.uni-lj.si/fn01leban/rn2007/
http://abra.fkkt.uni-lj.si/fn01leban/rn2008/
Weekly column in daily newspaper Dnevnik – "Science for All"
http://abra.fkkt.uni-lj.si/fn01leban/dnevnik/

SOME COMMENTS

There is a distinction between fundamental and applied research. Fundamental research at the university is necessary for undergraduate and graduate study programmes. It is also very tricky to forecast the results of investigations. Eventually, after some time, the results of fundamental research lead to application. Therefore, basic research at the university is a good foundation for innovative and R&D work for our graduates after they finish their studies. Our research is strongly connected with the study programmes of our faculty (Chemistry, Chemical Technology, Biochemistry). We have to point out also the difficulties we are facing. There is a strong tendency in Slovenia to apply an old model – i.e. to separate higher education (universities) and research (to be performed by research institutes). Also the Bologna reform goes in that direction – the first and second cycle vocationally oriented (more practical skills) while the real research degree is only achieved by a PhD. More and more PhD works nowadays are performed at research institutes which are also better equipped with research facilities. More outstanding PhD students take employment at the research institutes and not at universities or industry. It is important to note that the future for the university depends on "properly and well financed research university" and that the research institutes should perform more applied research for the industry. Education and research at universities are inseparable. It is worth mentioning that recently the University of Karlsruhe and Forschungszentrum Karlsruhe joined together to form an "elite university" with to achieve a large enough "critical mass." For that reason we should perform a proper "external" analysis of our higher education as well as research area and carefully consider all the recommendations.

It would be most helpful to have all the relevant data about higher education as well as for research on the internet. After all, we are obliged to deliver these data to EUROSTAT.

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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Tatjana Stipanovič

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

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

OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

Glede na zastavljene cilje je raziskovalno delo potekalo na naslednjih področjih:

1. Nove metode za sintezo funkcionaliziranih heterocikličnih spojin:
2. Nove metode in reagenti v stereoselektivni in asimetrični sintezi:
3. Kombinatorna sinteza heterocikličnih spojin
4. Sinteza indolovih alkaloidov in analogov na osnovi enaminonske metodologije
5. Sinteza novih heterocikličnih sistemov

1. NOVE METODE ZA SINTEZO FUNKCIONALIZIRANIH HETEROCIKLIČNIH SPOJIN

Študirali smo nove sintezne metode in pristope za pripravo funkcionaliziranih heterocikličnih spojin, ki vsebujejo terpensko, etilaminsko, amino kislinsko, dipeptidno, amino alkoholno in sorodne strukturne enote. Naša metodologija je vključevala predvsem sintezne pristope, ki temeljijo na primarni pripravi ustrezno funkcionaliziranih (acikličnih) prekurzorjev, ki ji nato sledi gradnja heterocikličnega obroča kot ključni korak sinteze ciljnega tipa spojin. Priprava prekurzorjev je temeljila na pretvorbi komercialno dostopnih izhodnih spojin po literaturnih postopkih oziroma po lastnih postopkih temelječih na splošnih principih organ-

ske sinteze. Za gradnjo heterocikličnih sistemov pa smo uporabljali predvsem dve splošni metodologiji:

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

V zvezi s sintezo funkcionaliziranih heterociklov velja izpostaviti naslednje dosežke:

– Sinteza (*S*)-3-pirazolilalaninov iz L-asparaginske kisline (*Synthesis* 2006, 2376–2384). Metoda vključuje štiristopenjsko pripravo β-keto estra, ki ga nato s formamid acetalom kvantitativno pretvorimo v optično aktivni enamino keton kot ključni intermediat (reagent). Sledi ciklokondenzacija reagenta z monosubstituiranimi hidrazini in hidrogenolitska odstranitev N- in O-zaščitnih skupin.
– Sinteza (2**R*,3**R*)-*N*-benzoil-3-cianobenzilidenamino-3-fenilalaninamidov iz (1*Z*,2**R*,5**R*)-4-benzoilamino-5-fenil-3-pirazolidinon-1-azometin iminov (*Tetrahedron Lett.* 2007, *48*, 5205–5208). Reakcije omenjenih azometin iminov so, presenetljivo, vodile do cepitve N–N vezi pirazolidinonskega obroča in nastanka zgoraj omenjenih spojin.
– Sinteza (*S*)-1-pirazolil-2-feniletilaminov iz L-fenilalanina in (1*S*,2*R*)-1-pirazolil-2-hidroksipropilaminov iz L-tirozina (*Helv. Chim. Acta* 2006, *89*, 30–44). Pri tej sintezni poti gre za večstopenjsko pretvorbo amino kisline v N-zaščiten Weinrebov amid, reakcijo z etinilmagnezijevim bromidom do ustreznega inona in sledečo konjugativno adicijo na trojno vez do ustreznega enamino ketona. Ciklokondenzacija enaminona s hidrazinovimi derivati in sledeča hidrogenolitska odstranitev N-zaščitne skupine vodi do končnih spojin.
– 'Ring switching' sinteza pirazolskih analogov histamina iz 2-pirolidinona (*Tetrahedron* 2007, *63*, 11213–11222). Gre za štiristopenjsko enostavno in učinkovito sintezo 2-(1-substituiranih 5-hidroksi-1*H*-pirazol-4-il)etilaminov, kjer 2-pirolidinon v dveh stopnjah pretvorimo v ustrezni N-benzoiliran α-enamino laktam, ki ga nato z 'ring switching' pretvorbo s hidrazinskim derivatom in sledečo hidrolizo pretvorimo v končne spojine.
– Sinteza N-substituiranih aminometilidentetramskih kislin iz L-fenilalanina in N-glicilglicina (*Synthesis* 2005, 2969–2988 Feature Article). Derivatizacija tetramskih kislin, pripravljenih iz L-fenilalanina in N-glicilglicina s formamid acetalom vodi do ustreznih enamino tetramatov. S sledečo izmenjavo dimetilaminske skupine z različnimi alifatskimi in (hetero)aromatskimi amini pa je bila pripravljena serija 50 3-(aminometiliden)tetramatov.
– Sinteza in pretvorbe terpenskih enaminonov so v zadnjih letih predstavljele pomembno področje našega delovanja. Pri tem smo iz (+)-kafre sintetizirali tri reagente, (1*R*,4*R*)-3-[(*E*)-(dimetilamino)metiliden]-1,7,7-trimetilbicyclo[2.2.1]heptan-2-o, njegov oksa homolog (*Tetrahedron: Asymmetry* 2004, *15*, 2367–2383) in njegov kamfolenolaktonski analog (*Tetrahedron: Asymmetry* 2006, *17*, 1715–1727). S temi reagenti smo študirali izmenjavo dimetilaminske skupine s C- in N-nukleofili (*Tetrahedron: Asymmetry* 2004, *15*, 2367–2383; *Synthesis* 2005,1087–1094; *Tetrahedron: Asymmetry* 2006, *17*, 1715–1727), ciklokondenzacije s hidrazini (*Tetrahedron* 2005, *61*, 3977–3990), nitroziranje s sledečo reakcijo z Grignardovimi reagenti (*Tetrahedron: Asymmetry* 2005, *16*, 2187–2197), sintezo diazenov in [1,2,4]triazolo[4,3-*x*]azinov s terpensko enoto (*Tetrahedron: Asymmetry* 2005, *16*, 2927–2945) in reakcije s 3-pirazolidinoni (*Acta. Chim.Slov.* 2006, *53*, 245–256).
– Sinteza bicikličnih pirazolidinonov kot heterocikličnih analogov dipeptidov na osnovi stereoselektivnih 1,3-dipolarnih cikloadicij (4*R**,5*R**)-4-benzoilamino-5-fenil-3-pirazolidinon-1-azometin iminov na različne dipolarofile (*Tetrahedron* 2005, *61*, 3991–3998; *Tetrahedron* 2007, *63*, 991–999; *J. Comb. Chem.* 2007, *9*, 717–723; *J. Heterocyclic Chem.*

2008, *45*, 181–188; *Z. Naturforsch.* 2008, *63b*, 375–383). Raziskave so vključevale študijo reaktivnosti različnih dipolov v reakcijah z različnimi dipolarofili z namenom ugotoviti selektivnost pretvorb pri sintezi različno substituiranih bicikličnih pirazolidinonov.

– Študirali smo[2+2]cikloadicije 2-amino-3-dimetilaminopropenoatov z acetilenkarboksilati pod vplivom mikrovalov. Pri tem so nastali polifunkcionalizirani derivati 1-amino-4-(dimetilamino)buta-1,3-dienov v 40–94 % izkoristkom. Pri vseh reakcijah je nastala samo ena izomerna oblika in tudi pri nesimetrično substituiranih acetilenih je reakcija potekala regiospecifično (*Tetrahedron Letters* 2008,*49,* 3775).
– Nove polisubstituirane (1*E*,3*E*)-1-(benzoilamino)-4-(dimetilamino)buta-1,3-diene-1,2,3-trikarboksilate smo uporabili kot vsestransko uporabne reagente v sintezi polisubstituiranih piridinov, *N*-aminopiridinov, pirolov in pirido[3,4-*c*]piridazinov. Tvorba določenega heterocikličnega sistema je odvisna od izhodnega (1*E*,3*E*)-1-(benzoilamino)-4-(dimetilamino)buta-1,3-dien-1,2,3-trikarboksilata. Z ustrezno izbiro estrske skupine lahko vodimo reakcijo v smer nastanka pirolovih ali piridinovih derivatov (*Tetrahedron* 2008, *64*, 9937–9946).
– Pripravili smo vrsto novih *N*-glikozidov (D-glukozide, D-manozide, L- and D-arabinozide, D-ksilozides in D-galaktozide), ki vsebujejo heterociklični aglikon, z reakcijo ustreznih heterocikličnih aminov s piranozami v metanolu. Strukturo spojin smo določili z ^{1}H in ^{13}C NMR spektorskopijo. Ugotovili smo, da v večini primerov spojine obstajajo v eni anomerni obliki (*Heterocycles* 2008, *75*, 2477–2491).
– Dietil (E)-4-[2-[2-(tert-butoksikarbonil)vinil]fenil]-2,6-dimetil-1,4-dihidropiridin-3,5-dikarboksilat (lacidipine) je zdravilo, ki se uporablja za zdravljenje visokega krvnega tlaka. Po vplivom dnevne in UV svetlobe poteka fototransformacija. Pri tem nastane 1α, 1aα,4aα,8bα,8cα) 1-(1,1-dimetil) 4,8c-dietill 1a,2,4a,8b-tetrahidro-1a,3-dimetill-2-azaciklobuta[jk]fluoren-1,4,8c(1H)-trikarboksilat. Strukturo smo določili z rentgenko analizo (*Acta Chim. Slov.* 2008, *55*, 458–461).
– Transformacije dialkil aceton-1,3-dikarboksilatov preko njihovih dimetilamino-metilidenskih derivatov v 1-substituirane 4-etoksikarbonil-5-(etoksikarbonilmetil)pirazole, 7-amino-2-etoksikarbonil-1*H*,2*H*-pirazolo[2,3-*c*]pirimidin-5-one, 4-hidroksipiridin-2(1*H*)-ones and 6-substituirane 3-benzoilamino-2,5-diokso-5,6-dihidro-2*H*-pirano[3,2-*c*]piridin-8-karbo-ksilate so opisane v *Acta Chim. Slov.* 2008, *55*, 1009–1018.
– Dva nova imidazo[1,2-*a*]piridina, 8-hidroksiimidazo[1,2-*a*]piridin -2-karboksilna kislina etil 8-hidroksiimidazo[1,2-*a*]piridin-2-karboksilat, sta bila pripravljena s ciklizacijo 2-aminopiridin-3-ol z bromopiruvično kislino in etil bromopiruvatom. 8-Hidroksiimidazo[1,2-*a*]piridin-2-karboksilna kislina je služila za pretvorbo z amino kislinami preko aktivni estrov v ustrezne biciklične sisteme (*Heterocycles* 2008, *75*, 1355–1370).

2. NOVE METODE IN REAGENTI V STEREOSELEKTIVNI IN ASIMETRIČNI SINTEZI

– Izvedena je bila sistematska študija modelnih 1,3-dipolarnih cikloadicij (4*R**,5*R**)-1-benziliden-4-benzoilamino-5-fenil-3-pirazolidinon-1-azometin iminov na modelne dipolarofile: dimetil maleat, dimetil fumarati in metil akrilat, ki je pokazala osnovne parametre, ki vplivajo na selektivnost in stereokemijo cikloadicij. Študija je pokazala odločujoč vpliv *orto*-substituentov aromatskega jedra azometin iminov na selektivnost in stereokemijo cikloadicij (*Tetrahedron* 2005, *61*, 3991–3998). V nadaljevanju smo študirali še cikloadicije na ostale tipične dipolarofile, kot so etil propiolat (*Z. Naturforsch.* 2008, *63b*, 375–383), maleimidi (*Tetrahedron* 2007, *63*, 991–999) in β-keti estri (*J. Comb. Chem.* 2007, *9*, 717–723). Pripravljena sta bila tudi dva predstavnika 1-alkiliden substituiranih azometin iminov, s katerima smo izvedli cikloadicije na značilne dipolarofile (*J. Heterocyclic Chem.* 2008, *45*, 181–188).

– Študirali smo tudi stereoselektivne redukcije α-heteroaril substituiranih kafer in njihovih oksa homologov (*Tetrahedron: Asymmetry* 2006, *17*, 79–91; *Tetrahedron: Asymmetry* 2007, *18*, 2365–2376), stereoselektivne [3+2]cikloadicije α-alkiliden kafer in sorodnih terpenskih sistemov (*Tetrahedron: Asymmetry* 2006, *17*, 1217–1237; *Tetrahedron: Asymmetry* 2007, *18*, 2365–2376) in [4+2] cikloadicije tetrazinov na eksociklično C=C vez 4'-metilenedihidro-3'*H*-spiro[biciklo[2.2.1]heptan-2,2'-furanov (*Tetrahedron: Asymmetry* 2007, *18*, 2746–2757). V večini primerov se je pokazalo, da je preferenčen sterično manj oviran *endo*-napad nukleofila oz. dipola ali diena. Pripravljeni so bili tudi novi kiralni ligandi salenskega tipa (*Tetrahedron: Asymmetry* 2004, *15*, 2367–2383) in stabilni prekurzorji ligandov karbenskega tipa (*Tetrahedron: Asymmetry* 2008,*19*, 330–342).
– Uporaba optično aktivnih diketopiperazinov kot kiralnih solvatacijskih reagentov v NMR spektroskopiji. Pri študiji sinteze dipodazinskih analogov so bile opažene kiralne solvatacijske lastnosti (*S*)-1-benzil-6-metilpiperazin-2,5-diona, ki omogočajo njegovo uporabo za določanje enantiomerne sestave in absolutne konfiguracije kiralnih amidov (*Tetrahedron: Asymmetry* 2007, *18*, 464–475; *Tetrahedron* 2008, *64*, 2801–2815; *Synthesis* 2008, 1436–1442).

3. KOMBINATORNA SINTEZA HETEROCIKLIČNIH SPOJIN

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

– Kombinatorna sinteza 3-arilamino-2,3-dehidroalaninov in njihovih analogov. Razvita je bila metoda v raztopini, ki omogoča enostavno izolacijo analitsko čistih produktov s filtracijo (*J. Comb. Chem.* 2004, *6*, 356–362).
– Kombinatorna sinteza kondenziranih 3-amino-4*H*-piridin-4-ov, 3-amino-4*H*-pirimidin-4-ov in 3-amino-2*H*-piran-2-onov kot heterocikličnih analogov amino kislin. Razviti sta bili obe osnovni varianti – sinteza v raztopini in sinteza na polimernem nosilcu. Sinteza v raztopini omogoča enostavno izolacijo analitsko čistih produktov (*J. Comb. Chem.* 2006, *8*, 95–102).
– Kombinatorna sinteza 4-acilaminopirolidin-5-on-2-karboksamidov v raztopini. Temelji na uporabi enaminonske metodologije za pripravo *terc*-butil (2*S*,4*S*)-2-amino-1-*terc*-butoksikarbonil-2-oksopirolidin-2-karboksilata kot ključnega reagenta. Sledi sekvenca selektivnih amidiranj in odstranitve zaščitnih skupin, ki vodi do knjižnic končnih produktov (*J. Comb. Chem.* 2007, *9*, 219–229).
– Kombinatorna sinteza bicikličnih pirazolidinonov kot heterocikličnih analogov dipeptidov. Na kombinatoren način smo v raztopini izvedli cikloadicije na maleimide (*Tetrahedron* 2007, *63*, 991–999) in β-keto estre (*J. Comb. Chem.* 2007, *9*, 717–723) in tako na enostaven način pripravili dve knjižnici analitsko čistih cikloaduktov.
– Razvili smo dve varianti na enaminonih osnovane paralelne sinteze na trdnih nosilcih 1-substituiranih 4-(2-aminoetill)-1*H*-pirazol-5-olov in njihovih NH-tavtomernih oblik. Sintezna strategija vsebuje dvostopenjsko pripravo *N*-zaščitenih α-enamino laktamov pripravljenih iz 2-pirolidinona ter »ring switching« pretvorbo z monosubstituiranimi hidrazini, in sledečo hidrolizo *N*-zaščitne skupine (*J. Comb. Chem.* 2008**,** *10*, 664–670).

4. SINTEZA INDOLOVIH ALKALOIDOV IN ANALOGOV NA OSNOVI ENAMINONSKE METODOLOGIJE

Pri študiju indolovih alkaloidov in sorodnih spojin smo sintetizirali vrsto 3-aril in 3-heteroaryl substituiranih indolovih derivatov (*Tetrahedron* 2004, *60*, 4601–4608) in meridianinskih

analogov (*Tetrahedron* 2005, *61*, 7508–7519). Uspelo nam je pripraviti tudi vrsto dipodazinskih analogov z enaminonsko sintezno metodologijo (*Helv. Chim. Acta* 2006, *89*, 240). Pri teh sintezah pa se je pojavil resen problem v zvezi z uvedbo kiralnega centra s (*S*)-alaninom v dipodazinske derivate. Epimerizacija te amino kisline poteče najverjetneje zaradi bazičnih pogojev pri reakciji s *tert*-butoksibis(dimetilamino)metanom. Z namenom, da bi se izognili tej epimerizaciji, smo izbrali vrsto alternativnih sintez, poleg tega pa smo pripravili tudi nov kiralni solvatacijski reagent, enantiomerno čisti (*S*)-1-benzil-6-metilpiperazin-2,5-dion (*Tetrahedron,* 2008, *64*, 2801–2815; *Tetrahedron: Asymmetry* 2007, *18*, 464–475). Sintetizirali smo tri sorodne diketopiperazine, (*S*)-1-benzil-6-metilpiperazin-2,5-dion, *S*)-1-benzil-3-metilpiperazin-2,5-dion, in *S*)-6-metill-1-(pentafluoro-benzil)piperazin-2,5-dion in jih uporabili kot potencialne kiralne solvatacijske reagente v NMR spektroskopiji (*Tetrahedron: Asymmetry* 2008, *19*, 1557–1567).

5. SINTEZA NOVIH HETEROCIKLIČNIH SISTEMOV

V sodelovanju z univerzo v Urbinu smo študirali reakcije 1,2-diaza-1,3-butadienov s 3-dimetilaminopropenoati. Pri tem so nastali novi pirolinski, pirolovi in oksazolinski derivati odvisno od reakcijskih pogojev in zaščiteni aziridini kondenzirani s pirolinskim obročem (O. A. Attanasi, G. Favi, P. Filippone, A. Golobič, B. Stanovnik, J. Svete, *J. Org. Chem.* 2005, *70*, 4307–4313). Poleg tega pa smo tudi študirali regio- in stereoselektivne sinteze piridazinov kondenziranih z oksazolini z Michaelovo adicijo-piridazinsko ciklizacijo-oksazolinsko ciklizacijo v kaskadnem sistemu 4-kloro-1,2-diaza-1,3-butadienov s 3-dimetilaminopropenoati (O. A. Attanasi, G. Favi, P. Filippone, A. Golobič, F. R. Perrulli, B. Stanovnik, J. Svete, *Synlett* 2006, 2971–2974). Izdelali smo tudi enostavno metodo za pripravo heteroaril-substituiranih pirimidinov (D. Bevk, U. Grošelj, A. Meden, J. Svete, B. Stanovnik, *Helv. Chim. Acta* 2007, *90*, 1737–1744).

6. PREGLEDNI ČLANKI

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3. J. Svete: Synthesis of functionalized compounds containing pyridazine and related moieties. *J. Heterocycl. Chem.* 2005, *42*, 361–373.
4. J. Svete: Utilization of chiral enaminones and azomethine imines in the synthesis of functionalized pyrazoles. *ARKIVOC*, 2006, part vii, 35–56.
5. D. Bevk, J. Svete, B. Stanovnik, Enaminones and related compounds in the synthesis of pyrazoles. In: *Modern Approaches to the Synthesis of O- and N-Heterocycles*, 2007, Vol. 3, 73–88. Eds. T. S. Kaufman, E. L. Larghi, Trivandrum, India.
6. B. Stanovnik, U. Grošelj, J. Svete, 1,2,4,5-Tetrazines. In: *Comprehensive Heterocyclic Chemistry III,* Eds.: A. R. Katritzky, C. A. Ramsden, E.F. V. Scriven, R. J. K. Taylor, Elsevier, Oxford, 2008, Vol. 9, pp. 641–713.
7. D. Kralj, J. Wagger, J. Svete, B. Stanovnik, Ethyl Isothiocyanatiacetate. ARTICLE – RN00838, Reagents in Organic Synthesis, 2008, v elektronski obliki

DRUGI RELEVANTNI DOSEŽKI

A) PLENARNA IN VABLJENA PREDAVANJA

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.

B) MEDNARODNE NAGRADE

B. Stanovnik:

a) 2006 "Kametani Award" for achievements in the field of heterocyclic chemistry awarded by "The Japan Institute of Heterocyclic Chemistry" (Tokyo, Japan) and Elsevier.

b) 2007 Medal and Diploma "In Memory of Professor A. N. Kost" awarded by the International Partership Foundation, Lomonosov Moscow State University and Mendeleev Russian Chemical Society, for achievements in the field of heterocyclic chemistry.

J. Svete, B. Stanovnik, U. Grošelj, D. Bevk, R. Jakše, A. Meden, S. Rečnik:

c) 2007 "Tetrahedron: Asymmetry Most Cited Paper 2004–2007 Award" for paper published in *Tetrahedron: Asymmetry* 2004, *15*, 2367–2383.

d) 2008 "Tetrahedron: Asymmetry Most Cited Paper 2005–2008 Award" for paper published in *Tetrahedron: Asymmetry* 2005, *16*, 2187–2197.

e) 2008 "Tetrahedron Most Cited Paper 2005–2008 Award" for paper published in *Tetrahedron* 2005*, 61*, 3991–3998.

C) ČLANSTVO MEDNARODNIH ZNANSTVENIH ODBOROV KONGRESOV IN SIMPOZIJEV IN DRUGE ADMINISTRATIVNE FUNKCIJE

B. Stanovnik:

a) Member of the Scientific Committee, European Colloquia of Heterocyclic Chemistry

b) Member of the Scientific Committee, Blue Danube Symposia of Heterocyclic Chemistry

c) Member of the Board of Electron Journal ARKIVOC

d) Member of the Advisory Board "Advances in Heterocyclic Chemistry"

e) Member of the Scientific Committee, TRAMECH Transmediterranean Symposia of Heterocyclic Chemistry

f) Member of the International Advisory Committee of the IBN SINA International Conferences on Pure and Applied Heterocyclic Chemistry

g) Member of the Scientific Committee of Eurasian Meetings on Heterocyclic Chemistry

h) Member of the Advisory Board, Trends in Heterocyclic Chemistry

i) Predstojnik Oddelka za mednarodno sodelovanje in znanstveno koordinacijo Slovenske akademije znanosti in umetnosti, Ljubljana, Slovenija

j) Dekan razreda za naravoslovne znanosti Evropske akademije znanosti, Salzburg, Austria

k) Member of the Advisory Board, Croatica Chemica Acta

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

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

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

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

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

The research work was carried out in the following fields:

1. New methods for the synthesis of functionalized heterocyclic compounds
2. New methods and reagents in stereoselective and asymmetric synthesis
3. Combinatorial synthesis of heterocyclic compounds
4. Synthesis of indole alkaloids and analogs by enaminone methodology
5. Synthesis of new heterocyclic systems

1. NEW METHODS FOR THE SYNTHESIS OF FUNCTIONALIZED HETEROCYCLIC COMPOUNDS

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

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

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

– Synthesis of (*S*)-3-pyrazolylalanines from L-aspartic acid (*Synthesis* 2006, 2376–2384) comprising a four-step preparation of functionalized β-keto ester, its transformation with formamide acetal into enamino ketone as the key-intermediate (reagent). Final compounds were obtained by cyclocondensation with monosubstituted hydrazines followed by hydrogenolytic deprotection.
– Synthesis of (2**R*,3**R*)-*N*-benzoyl-3-cyanobenzylideneamino-3-phenylalaninamides from (1*Z*,2**R*,5**R*)-4-benzoylamino-5-phenyl-3-pyrazolidinon-1-azomethine imines (*Tetrahedron Lett.* 2007, *48*, 5205–5208). Surprisingly, reactions of azomethine imines with HCN gave the title compounds as a consequence of N–N bond fission.
– Synthesis of (*S*)-1-pyrazolyl-2-phenylethylamines from L-phenylalanine and (1*S*,2*R*)-1-pyrazolyl-2-hydroxypropylamines from L-tyrozine (*Helv. Chim. Acta* 2006, *89*, 30–44).

Amino acid is transformed into the corresponding N-protected Weinreb amide which reacted with ethinylmagnesium bromide to give the corresponding ynone, followed by conjugative addition of a secondary amine to the triple bond to furnish the enamino ketone. Subsequent cyclization with hydrazine derivatives and hydrogenolytic deprotection gave the title compounds.

– 'Ring switching' synthesis of pyrazole analogues of histamine from 2-pyrrolidinone (*Tetrahedron* 2007, *63*, 11213–11222). A four-step, simple and efficient synthesis of 2-(1-substituted 5-hydroxy-1*H*-pyrazol-4-yl)ethylamines, where 2-pyrrolidinone is transformed in two steps into enamino lactam as the key-intermediate was developed. 'Ring switching' transformation of enamino lactam with hydrazine derivatives followed by hydrolytic deprotection leads to the title compounds.
– Synthesis of N-substituted aminomethylidenetetramic acids from L-phenylalanine in N-glycylglycine (*Synthesis* 2005, 2969–2988 Feature Article). Derivatives of tetramic acids, prepared from L-phenylalanine and N-glycylglycine with formamide acetal, were transformed to the corresponding enamino tetramates. A series of 50 aminomethylidene tetramates was prepared by treatment with aliphatic and (hetero)aromatic amines.
– Synthesis and transformations of terpene functionalized enaminones were also the subject of our research. Starting from (+)-camphor, three reagents were synthesized, (1*R*,4*R*)-3-[(*E*)-(dimethylamino)methylidene]-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one, its oxa homologue (*Tetrahedron: Asymmetry* 2004, *15*, 2367–2383), and its campholenolactone analogue (*Tetrahedron: Asymmetry* 2006, *17*, 1715–1727). The following reactions were carried out with these three reagents: substitution of the dimethylamino group with C- and N-nucleophiles (*Tetrahedron: Asymmetry* 2004, *15*, 2367–2383; *Synthesis* 2005,1087–1094; *Tetrahedron: Asymmetry* 2006, *17*, 1715–1727), cyclocondensations with hydrazines (*Tetrahedron* 2005, *61*, 3977–3990), nitrosation followed by treatment with Grignard reagents (*Tetrahedron: Asymmetry* 2005, *16*, 2187–2197), synthesis of diazenes and [1,2,4]triazolo[4,3-*x*]azines attached to terpene unit (*Tetrahedron: Asymmetry* 2005, *16*, 2927–2945), and reactions with 3-pyrazolidinones (*Acta. Chim.Slov.* 2006, *53*, 245–256).
– Synthesis of bicyclic pyrazolidinones as heterocyclic analogues based on 1,3-dipolar cycloadditions of (4*R**,5*R**)-4-benzoylamino-5-phenyl-3-pyrazolidinon-1-azomethine imines to various dipolarophiles (*Tetrahedron* 2005, *61*, 3991–3998; *Tetrahedron* 2007, *63*, 991–999; *J. Comb. Chem.* 2007, *9*, 717–723; *J. Heterocyclic Chem.* 2008, *45*, 181–188; *Z. Naturforsch.* 2008, *63b*, 375–383). This was a basic study on reactivity, selectivity, and stereochemistry of these cycloadditions with intention to determine the reactivity and selectivity pattern in the synthesis of bicyclic pyrazolidinones.
– Microwave assisted [2+2] cycloaddition reactions of 2-amino-3-dimethylaminopropenoates with acetylenecarboxylates furnished highly functionalised 1-amino-4-(dimethylamino)buta-1,3-dienes with 40–94% yields. All reactions were observed to consistently produce single geometrical isomers and also in cases, where non-symmetrical acetylenes were engaged, the reactions proceeded in a regiospecific manner. (*Tetrahedron Letters* 2008, *49,* 3775).
– New highly functionalized (1*E*,3*E*)-1-(benzoylamino)-4-(dimethylamino)buta-1,3-diene-1,2,3-tricarboxylates proved to be useful and versatile reagents in the formation of highly substituted pyridine, *N*-aminopyridine, pyrrole and pyrido[3,4-*c*]pyridazine derivatives. The formation of a particular type heterocyclic system depends on the starting (1*E*,3*E*)-1-(benzoylamino)-4-(dimethylamino)buta-1,3-diene-1,2,3-tricarboxylate. By an appropriate choice of different ester groups it is possible to drive the reactions towards the formation of either pyridine or pyrrole derivatives. (*Tetrahedron* 2008, *64*, 9937–9946).

– A series of new *N*-glycosides (D-glucosides, D-mannosides, L- and D-arabinosides, D-xylosides and one D-galactoside) containing heterocyclic moiety have been prepared by the reaction of corresponding heterocyclic amines with pyranoses in boiling methanol. The structures of the prepared compounds have been studied by means of proton and carbon NMR spectroscopy. In most cases the products existed in DMSO solution as single anomers. (*Heterocycles* 2008, *75*, 2477–2491).
– Diethyl(*E*)-4-[2-[2-(tert-butoxycarbonyl)vinyl]phenyl]-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate or lacidipine (**1**) is a drug used for the treatment of hypertension. The literature data for the undesired daylight phototransformation of compound **1** was confirmed for UV light as well. The main product, (1α, 1aα,4aα,8bα,8cα) 1-(1,1-dimethylethyl) 4,8c-diethyl 1a,2,4a,8b-tetrahydro-1a,3-dimethyl-2-azacyclobuta[jk]fluorene-1,4,8c(1*H*)-tricarboxylate was isolated and crystal structure was determined by X-ray analysis of a monocrystal. (*Acta Chim. Slov.* 2008, *55*, 458–461).
– Transformations of dialkyl acetone-1,3-dicarboxylates *via* their dimethylaminomethylidene derivatives into 1-substituted 4-ethoxycarbonyl-5-(ethoxycarbonylmethyl)pyrazoles, 7-amino-2-ethoxycarbonyl-1*H*,2*H*-pyrazolo[2,3-*c*]pyrimidin-5-one, 4-hydroxypyridin-2(1*H*)-ones and 6-substituted 3-benzoylamino-2,5-dioxo-5,6-dihydro-2*H*-pyrano[3,2-*c*]pyridine-8-carboxyla-tes are described in *Acta Chim. Slov.* 2008, *55*, 1009–1018.
– Two new imidazo[1,2-*a*]pyridines, 8-hydroxyimidazo[1,2-*a*]pyridine -2-carboxylic acid and ethyl 8-hydroxyimidazo[1,2-*a*]pyridine-2-carboxylate, were prepared *via* cyclization of 2-aminopyridin-3-ol with bromopyruvic acid and ethyl bromopyruvate, respectively. 8-Hydroxyimidazo[1,2-*a*]pyridine-2- carboxylic acid was successfully coupled with various amino acid derivatives *via* its active ester intermediate into the corresponding amides. *O*-protected ethyl 8-hydroxyimidazo[1,2-*a*]pyridine-2-carboxylate was transformed into its hydrazide and amide derivatives. (*Heterocycles* 2008, *75*, 1355–1370).

2. NEW METHODS AND REAGENTS IN STEREOSELECTIVE AND ASYMMETRIC SYNTHESIS

– A systematic study on 1,3-dipolar cycloadditions of (4*R**,5*R**)-1-benzylidene-4-benzoylamino-5-phenyl-3-pyrazolidinon-1-azomethine imines as model dipoles to model dipolarophiles: dimethyl maleate, dimethyl fumarate, and methyl acrylate was performed. This study showed some basic parameters which influence the selectivity and stereochemistry of cycloadditions. The study also showed that *ortho*-substituents at the aryl group of azomethine imines control the selectivity and stereochemistry of cycloadditions (*Tetrahedron* 2005, *61*, 3991–3998). In addition to this, reactions with some other typical dipolarophiles, such as ethyl propiolate (*Z. Naturforsch.* 2008, *63b*, 375–383), maleimides (*Tetrahedron* 2007, *63*, 991–999), and β-keto esters (*J. Comb. Chem.* **2**007, *9*, 717–723) were carried out. Two representatives of 1-alkylidene substituted azomethine imines were also prepared and used in cycloadditions to typical dipolarophiles (*J. Heterocyclic Chem.* 2008, *45*, 181–188).
– Stereoselective reductions of α-alkylidene-(+)-camphors and their oxa analogues (*Tetrahedron: Asymmetry* 2006, *17*, 79–91; *Tetrahedron: Asymmetry* 2007, *18*, 2365–2376), stereoselective [3+2] cycloadditions to α-alkylidene-(+)-camphors and related systems (*Tetrahedron: Asymmetry* 2006, *17*, 1217–1237; *Tetrahedron: Asymmetry* 2007, *18*, 2365–2376), and [4+2] cycloadditions of tetrazines to exocyclic C=C bond in 4'-methylenedihydro-3'*H*-spiro[bicyclo[2.2.1]heptan-2,2'-furans (*Tetrahedron: Asymmetry* 2007, *18*, 2746–2757) were also carried out. In most cases, these reactions were *endo*-selective, due to sterically less hindered *endo*-approach of the dipole or diene. New salen-type chiral ligands (*Tetrahedron: Asymmetry* 2004, *15*, 2367–2383) and new precursors for chiral N-heterocyclic carbenes (*Tetrahedron: Asymmetry* 2008,*19*, 330–342) were also synthesized.

– Utilization of non-racemic diketopiperazines a chiral solvating agents (CSA) in NMR spectroscopy. In the course of our studies on the synthesis of dipodazine analogues, chiral solvating properties of (*S*)-1-benzyl-6-methylpiperazine-2,5-dione were observed and studied. These properties make it possible to use such diketopiperazines for the determination of ee and absolute configuration of chiral amides by NMR spectroscopy, especially in connection with the synthesis of trypropstans A and B and their analogs. (*Tetrahedron: Asymmetry* 2007, *18*, 464–475; *Tetrahedron* 2008, *64*, 2801–2815; *Synthesis* 2008, 1436–1442).

3. COMBINATORIAL SYNTHESIS OF HETEROCYCLIC COMPOUNDS

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

– Combinatorial solution-phase synthesis of 3-arylamino-2,3-dehydroalanines and their analogues, which includes a simple filtration workup and isolation of analytically pure products (*J. Comb. Chem.* 2004, *6*, 356–362).
– Combinatorial synthesis of fused 3-amino-4*H*-piridin-4-ones, 3-amino-4*H*-pirimidin-4-ones, and 3-amino-2*H*-piran-2-ones as heterocyclic analogues of amino acids. Both variants were developed – a solution-phase synthesis and a solid-phase synthesis. Synthesis in solution enables a simple isolation of analytically pure products (*J. Comb. Chem.* 2006, *8*, 95–102).
– Combinatorial solution-phase synthesis of 4-acylaminopyrrolidin-2-one-4-carboxamides *via* enaminone-based synthesis of *tert*-butyl (2*S*,4*S*)-2-amino-1-*tert*-butoxycarbonyl-2-oxopyrrolidin-2-carboxylate as the key-intermediate. A sequence of amidation and deprotection steps then leads to a library of target compounds (*J. Comb. Chem.* 2007, *9*, 219–229).
– Combinatorial synthesis of bicyclic pyrazolidinones as heterocyclic analogues of dipeptides. Combinatorial cycloadditions of azomethine imines to maleimides (*Tetrahedron* 2007, *63*, 991–999) and β-keto esters (*J. Comb. Chem.* 2007, *9*, 717–723) gave libraries of analytically pure products upon simple workup protocol.
– Two variations of enaminone-based parallel solution-phase synthesis of 1-substituted 4-(2-aminoethyl)-1*H*-pyrazol-5-ols and their NH-tautomers were developed. The synthetic strategy comprises a two step preparation of the *N*-protected α-enamino lactams from 2-pyrrolidinone, “ring switching” transformation with monosubstituted hydrazines, and acidolytic removal of the *N*-protecting group.(*J. Comb. Chem.* 2008, *10*, 664–670).

4. SYNTHESIS OF INDOLE ALKALOIDS AND ANALOGS BY ENAMINONE METHODOLOGY. SYNTHESIS AND APPLICATIONS OF NEW CHIRAL SOLVATING AGENTS

In the field of indole alkaloids and related compounds a series of 3-aryl and 3-heteroaryl substituted indole derivatives (*Tetrahedron* 2004, *60*, 4601–4608) and meridianine analogs (*Tetrahedron* 2005, *61*, 7508–7519) have been prepared. We have been also successful in preparation of a series of dipodazin analogs by the same method (*Helv. Chim. Acta* 2006, *89*, 240). However, in this research a serious problem has been encountered in connection with introduction of a chiral center with (*S*)-alanine into the dipodazine molecule. Epimerization of the chiral center of this molecule is most probably due to the basic conditions in the reaction with *tert*-butoxybis(dimethylamino)methane. In order to avoid this epimerization, a number of alternative syntheses have been selected and a new chiral solvating reagent has been prepared. This reagent is enantiomerically pure (*S*)-1-benzyl-6-methylpiperazine-2,5-dione (*Tetrahedron,* 2008, *64*, 2801–2815; *Tetrtahedron: Asymmetry* 2007, *18*, 464–475. Three closely

related diketopiperazines, (*S*)-1-benzyl-6-methylpiperazine-2,5-dione, *S*)-1-benzyl-3-methylpiperazine-2,5-dione, and *S*)-6-methyl-1-(pentafluorobenzyl)piperazine-2,5-dione were prepared and screened as potential chiral solvating agents in NMR spectroscopy. (*Tetrahedron: Asymmetry* 2008, *19*, 1557–1567).

5. SYNTHESIS OF NEW HETEROCYCLIC SYSTEMS

In cooperation with the University of Urbino the reactions of 1,2-diaza-1,3-butadines with 3-dimethylaminopropenoates have been studied. New pyrroline, pyrrole and oxazoline derivatives were isolated, dependent on reaction conditions and aziridines condensed with pyrroline system (O. A. Attanasi, G. Favi, P. Filippone, A. Golobič, B. Stanovnik, J. Svete, *J. Org. Chem.* 2005, *70*, 4307–4313). Regio- and stereoslective reactions of pyridazines condensed with oxazoline system were prepared by "Michael addition – pyridazine cyclization – oxazoline cyclization cascade reaction of 4-chloro-1,2-diaza-1,3-butadienes with 3-dimethylaminopropenoates (O. A. Attanasi, G. Favi, P. Filippone, A. Golobič, F. R. Perrulli, B. Stanovnik, J. Svete, *Synlett* 2006, 2971–2974). A new simple synthesis for preparation of heteroaryl-substituted pyrimidines has been developed (D. Bevk, U. Grošelj, A. Meden, J. Svete, B. Stanovnik, *Helv. Chim. Acta* 2007, *90*, 1737–1744.

6. REVIEW ARTICLES

1. B. Stanovnik, J. Svete: Synthesis of heterocycles from alkyl 3-(dimethylamino)propenoates and related enaminones. Chem. Rev. 2004, 104, 2433–2480. (IF ~ 21, the highest IF in chemistry).
2. J. Svete: Ex-chiral ppol enaminones in the synthesis offunctional heterocycles. *Monatsh. Chem.* 2004, *135*, 629–647.
3. J. Svete: Synthesis of functionalized compounds containing pyridazine and related moieties. *J. Heterocycl. Chem.* 2005, *42*, 361–373.
4. J. Svete: Utilization of chiral enaminones and azomethine imines in the synthesis of functionalized pyrazoles. *ARKIVOC*, 2006, part vii, 35–56.
5. D. Bevk, J. Svete, B. Stanovnik, Enaminones and related compounds in the synthesis of pyrazoles. In: *Modern Approaches to the Synthesis of O- and N-Heterocycles*, 2007, Vol. 3, 73–88. Eds. T. S. Kaufman, E. L. Larghi, Trivandrum, India.
6. B. Stanovnik, U. Grošelj, J. Svete, 1,2,4,5-Tetrazines. In: *Comprehensive Heterocyclic ChemistryIII,* Eds.: A. R. Katritzky, C. A. Ramsden, E.F. V. Scriven, R. J. K. Taylor, Elsevier, Oxford, 2008, Vol. 9, pp. 641–713.
7. D. Kralj, J. Wagger, J. Svete, B. Stanovnik, Ethyl Isothiocyanatiacetate. ARTICLE – RN00838, Reagents in Organic Synthesis, 2008, v electronski obliki

OTHER RELEVANT ACHIEVEMENTS

A PLENARY AND INVITED LECTURES

Members of the research group delivered several plenary and invited lectures at international congresses and symposia, and at various universities. They obtained some international awards. The details are given in the report of the Chair of Organic Chemistry.

B INTERNATIOANL AWARDS

B. Stanovnik:

a) 2006 “Kametani Award” for achievements in the field of heterocyclic chemistry awarded by “The Japan Institute of Heterocyclic Chemistry” (Tokyo, Japan) and Elsevier.

b) 2007 Medal and Diploma “In Memory of Professor A. N. Kost” awarded by the International Partership Foundation, Lomonosov Moscow State University and Mendeleev Russian Chemical Society, for achievements in the field of heterocyclic chemistry.

J. Svete, B. Stanovnik, U. Grošelj, D. Bevk, R. Jakše, A. Meden, S. Rečnik:

c) 2007 “Tetrahedron: Asymmetry Most Cited Paper 2004–2007 Award” for the paper published in *Tetrahedron: Asymmetry* 2004, *15*, 2367–2383.

d) 2008 “Tetrahedron: Asymmetry Most Cited Paper 2005–2008 Award” for the paper published in *Tetrahedron: Asymmetry* 2005, *16*, 2187–2197.

e) 2008 “Tetrahedron Most Cited Paper 2005–2008 Award” for the paper published in *Tetrahedron* 2005*, 61*, 3991–3998.

C MEMBERSHIP IN SCIENTIFIC COMMITTEES OF INTERNATIONAL CONFERENCES AND SYMPOSIA AND OTHER ADMINISTRATIVE FUNCTIONS

B. Stanovnik:

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

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

c) Member of the Advisory Board, Croatica Chemica Acta, Croatia

d) Member of the Scientific Committee, European Colloquia of Heterocyclic Chemistry

e) Member of the Scientific Committee, Blue Danube Symposia of Heterocyclic Chemistry

f) Member of the Advisory Editorial Board, Journal of Heterocyclic Chemistry, USA

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

h) Member of the Board of Electronic Journal ARKIVOC

i) Head, Department of International Relations and Scientific Coordination of the Slovenian Academy of Sciences and Arts

j) Member of the Advisory Board, Advances in Heterocyclic Chemistry

k) Member of the Scientific Committee of TRAMECH Symposia (Transmediterranean Symposia of Heterocyclic Chemistry)

l) Member of the International Advisory Committee of Ibn Sina International Conferences On Pure and Applied Heterocyclic Chemistry, Egypt

m) Decanus Classis Scientiarum Naturalium Academiae Scientiarum et Artium Europeae, Salzburg. (Dean of the Class “Natural Sciences” of the European Academy of Sciences and Arts, Salzburg)

n) Member of the Scientific Committee of the Eurasian Meeting on Heterocyclic Chemistry

o) Member of the Advisory Editorial Board, Trends in Heterocyclic Chemistry

FIZIKALNA KEMIJA
PHYSICAL CHEMISTRY

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P1–0201

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prof. dr. Vojeslav Vlachy

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prof. dr. Ciril Pohar
doc. dr. Jurij Reščič
prof. dr. Jože Škerjanc
dr. Matija Tomšič
doc. dr. Tomaž Urbič
prof. dr. Gorazd Vesnaver
prof. dr. Vojeslav Vlachy

Mladi raziskovalci / Young Researchers
Alan Bizjak
Igor Drobnak
Boštjan Jerman
Martin Tine Perger
Iztok Prislan
Mario Šimić
Andrej Lajovic

Tehniki / Technicians
Anton Kelbl
Anton Kokalj
Cirila Peklaj

POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

Naše raziskave prispevajo k razumevanju fizikalno–kemijskih procesov, ki se dogajajo v živih bitjih in/ali so pomembni v industriji. Zanimajo nas raztopine in suspenzije nanodelcev, predvsem polielektrolitov. Nekateri od njih so biološko pomembni (proteini in DNK), drugi, na primer, površinsko aktivne snovi in sintetični polielektroliti pa se na široko uporabljajo v industriji. Raziskave stabilnosti proteinov in DNK, vezave ligandov na DNK in podobnosti molekul so pomembne v farmacevtski industriji in bioinženirstvu; prav na teh področjih sodelujemo tudi z industrijo. Eksperimentalne raziskave se dopolnjujejo s teoretičnimi; namen našega dela je boljše razumevanje procesov na molekularnem nivoju in posredovanje tega znanja študentom ter kolegom v industriji. V času trajanja programa smo objavili 141 člankov v uglednih znanstvenih revijah, kot so Annu. Rev. Biophys. Biomol. Struc. (IF:16,2; od l. 2005 56 neodvisnih citatov), Biochemistry&Molecular biol. (IF:13,3), J. Am. Chem. Soc. (IF:7,9), Nucleic Acids Res., (IF: 6.95), J. Biol. Chem. (IF: 5.8), Curr. Opin. Coll. Interface Sci. (IF:5,3), J. Phys. Chem B, J. Chem. Phys., Langmuir, Chem. Phys. Letters in druge. Objavili smo tudi tri prispevke v monografskih publikacijah. Zaradi pomanjkanja prostora smo v nadaljevanju navedli le nekatera dela. Citiranje je v skladu z bibliografijo navedeno v Sicrisu za obdobje od leta 2004 do 2008.

OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

1. Teoretične in eksperimentalne raziskave disperznih sistemov. Z računalniško simulacijo Monte Carlo (MC), teorijo na osnovi gostotnega funkcionala ter z integralskimi enačbami smo proučevali lastnosti modelnih tekočin v homogenih sistemih ter pod vplivom zunanjega polja [21,22,47,57,62–64,79,81,92,112,120]. Z metodo ozkokotnega rentgenskega sipanja in dinamičnega sipanja laserske svetlobe smo raziskovali strukturne in dinamične lastnosti samo-organiziranih sistemov [6,10, 52, 55], biološko pomembnih sistemov [5, 33, 43], strukturiranih topil [71, 91] in gelirnih polisaharidov [114]. Študirali smo (in–vitro) sproščanje

modelne učinkovine iz mikroemulzije [18,52]. Glej tudi: M. Tomšič in A. Jamnik, *Simple Alcohols and their Role in Structure and Interactions of Microemulsion Systems* (poglavje 6) in M. Gašperlin in M. Bešter−Rogač, *Physicochemical Characterization of Pharmaceutically Applicable Microemulsions: Tween 40/Imwitor 308/Isopropyl Myristate/Water* (poglavje 10), V Monzer Fanun (Ed.) Microemulsions: Properties and Applications, CRC Press, Taylor & Francis, 2008. Raziskovali smo [9,39,72,75,93] porazdelitev ionov med nanoporoznoznim adsorbentom in nemoteno raztopino.

2. Elektroliti in polielektroliti. Ugotovili smo, da v vodni raztopini sulfatov dvovaletnih kovin obstajajo tri vrste ionskih parov [26, 90, 99,110]. Pri študiju heksakarboksilne benzenove kisline in njenih kislih ter nevtralnih soli smo uporabili Quint–Viallard enačbe za opis disociacijskih in hidroliznih ravnotežij [58]. Raziskovali smo lastnosti vodnih raztopin nabitih alkalijskih fulerenheksamalonatov [42,87,117,119]. Izmerili smo osmozni tlak in razredčilne toplote raztopin [95] polianetolesulfonske kisline in njenih alkalijskih soli. Z določanjem koncentracijske odvisnosti razredčilnih entalpij poliglutaminske kisline smo raziskali konformacijski prehod med vijačnico in klobčičem [29]. Če raztopini elektrolita dodamo polielektrolit se reakcija med protiioni močno pospeši. Ta efekt, smo teoretično raziskali v delih [31,40,84,101,111]. Med teoretičnimi raziskavami so pomembne simulacije raztopin verižnih polielektrolitov [54], kjer smo raziskali korelacijo med dolžino polielektrolita in osmoznim tlakom, študij interakcije med paličastimi protioini in sferičnimi poliioni [118] in vpliv dielektrične nezveznosti [133] na interakcijo med koloidi. Študirali smo vpliv stereoregularnosti na lastnosti polimetakrilne kisline. Pokazali smo [11,37,73,94, 143], da stereoregularna sestava vpliva na termodinamične lastnosti PMA.

3. Površinsko aktivne snovi (PAS). Študirali smo interakcije med PAS in nasprotno nabitimi polielektroliti ali poliamfoliti, nasprotno nabitimi derivati fulerena in fosfolipidnimi membranami [25,32,59,69,74,89,97]. Za določitev stopnje vezanja smo uporabili PAS ion–selektivne membrane. Z merjenjem električne prevodnosti vodnih raztopin alikiltrimetilamonijevih kloridov z različno dolžino alkilne verige smo proučevali proces micelizacije [60, 88,121].

4. Industrijsko pomembni topljenci. Soli cikloheksilsulfaminske kisline, kalijev acesulfam in natrijev saharin so umetna sladila. Z merjenjem električne prevodnosti smo ugotovili, da so le–ta v vodi popolnoma ionizirana kar verjetno vpliva na interakcije z receptorji okusa [30, 41,122]. V razredčenih vodnih raztopinah penicilin G natrijeve in kalijeve soli ter penicilin V kalijeve soli kažejo lastnosti kislih soli dvobaznih kislin [96].

5. Hidratacija preprostih in sestavljenih topljencev [3,128,133]. Raziskovali smo hidratacijo ionov in nepolarnih delcev [8,36,76, 85,86]. Uporabili smo metodo Monte Carlo, molekulsko dinamiko (MD) in teorije na osnovi Wertheimove Ornstein–Zernike integralske enačbe. Študirali smo vedenje modelne vode v zaprtih sistemih [56]. Raziskovali smo hidratacijo polielektrolitov [78]. V delu [107] smo uporabili metodo MD, da bi raziskali vpliv vrste iona na interakcijo med kvarternim dušikom na oligomeru ionena in protioni v raztopini.

6. Kvantna kemija in molekulska podobnost. Interakcijo molekule netropsina z DNK, smo obravnavali s simulacijo dinamike molekul [20, 28]. Pri vezavi netropsina in distamicina v ožji kanal DNK [34] pa smo študirali pomembnost spremembe konfiguracijske entropije. Na področju molekulske podobnosti smo razvili nove deskriptorje na osnovi primerjave indirektnih (RDF) zapisov molekul [12, 61]. Sodelovali smo pri razvoju učinkovin zoper kolero [65,77,135].

7. Raziskave biološko pomembnih molekul [134]. Prispevali smo k razlagi pojavov na področju molekulskega prepoznavanja nukleinskih kislin z majhnimi molekulami [126]. Na osnovi študija interakcij protein–protein in protein–DNA smo objavili pregled odkritij s področja bak-

terijske celične smrti [134]. Uspeli smo povezati termodinamiko razvitja fleksibilnega (nativno nerazvitega) proteina z celično smtrjo pri bakterijah [19]. V drugem primeru smo raziskali povezavo med termodinamiko in strukturnimi lastnostmi eritropoietina [14]. Razlage zapletenih biomolekularnih procesov temeljijo na modelih, ki smo jih preverjali na procesu micelizacije površinsko aktivne snovi [60]. Uspelo nam je izdelati model, ki s samo pozitivnimi aktivacijskimi energijami za vse elementarne reakcije, uspešno opiše zvijanje in razvijanje nekaterih G-kvadrupleksov [124]. V nizu teoretičnih in eksperimentalnih del smo določali lastnosti mešanic proteinov z navadnim elektrolitom oziroma z nevtralnim polimerom [43,53,83]. Določili smo topnost lizocima v prisotnosti nekaterih soli in PEG [106].

8. Kristalizacija. Obarjanje nekaterih industrijsko pomembnih produktov smo raziskali v delih [1,24,49].

DRUGI RELEVANTNI DOSEŽKI

1. Imeli smo eno plenarno predavanje in več uvodnih predavanj na mednarodnih konferencah doma in v tujini. O svojem delu smo poročali na mnogih tujih univerzah in inštitutih kot so UC San Francisco, University of Coimbra, UC San Juan PR, University of Regensburg, Paul Scherrer Institute Villigen, University of Queensland, Brisbane, University Pierre and Marie Curie Paris, CEA (Saclay), Uppsala University, Institut d'Investigacions Químiques i Ambientals de Barcelona in še na nekaterih drugih ustanovah doma in v tujini.

2. Organizirali smo 29. International Conference on Solution Chemistry, ki je potekala od 20. do 25. 8. 2005 v Portorožu. Predsednik prireditvenega odbora je bil V. Vlachy, sekretarka pa M. Bešter Rogač. Častna pokroviteljica je bila Mednarodna zveza za čisto in uporabno kemijo (I.U.P.A.C). Število udeležencev je bilo okoli 300, prišli so iz 37 držav sveta. Med predavatelji je bil tudi Nobelov nagrajenec profesor Jean–Marie Lehn.

3. V. Vlachy in M. Bešter Rogač sta bila vabljena urednika pri Pure and Applied Chemistry (vol. 78, 2006, št. 8) in Journal of Molecular Liquids (vol. 131−132, str. 1−254, 2007).

4. M. Bešter Rogač je sourednica Acta Chimica Slovenica in Journal of Molecular Liquids (Elsevier).

5. V. Vlachy je bil izvoljen za rednega člana Evropske akademije znanosti in umetnosti.

6. A. Godec je bil med dobitniki priznanja Slovenske znanstvene fundacije *Prometej znanosti za odličnost v komuniciranju* za leto 2008.

7. Člani programske skupine so bili večkrat mentorji študentom, ki so dobili Prešernove (univerzitetne in fakultetne) nagrade ter Krkine nagrade.

8. Več članov PS je bilo v tem obdobju na študijskem izpopolnjevanju (vsaj 3 mesece) v tujini (Jožica Dolenc –ETH Zürich, A. Bizjak – UC San Francisco, Miha Lukšič – University of Regensburg, Matjaž Bončina – Max–Planck Institut für Polymerforschung, Mainz).

9. V šolskem letu 2006/07 je bil V. Vlachy tri mesece gostujoči profesor na UC San Francisco, 6-mesecev na Univerzi v Regensburgu in en mesec na Université Pierre et Marie Curie, Pariz–6, Francija.

10. V. Vlachy je bil na "Department of Pharmaceutical Chemistry, University of California, San Francisco" ponovno izvoljen v naziv "Adjunct Professor."

11. Sodelovali smo in še sodelujemo v bilateralnih projektih z Avstrijo, Madžarsko, Hrvaško, Portugalsko, ZDA, Francijo in Ukrajino.

12. Kot partnerji univerze v San Franciscu že osem let sodelujemo pri projektu "Solvation in Biology", ki ga financira National Institute of Health, ZDA.

13. Sodelujemo tudi pri dveh COST projektih (D–31 G. Vesnaver, D–43 M. Bešter Rogač), imamo en podoktorski projekt (J. Dolenc, »Simulacije molekulske dinamike nukleinskih kislin: struktura, dinamika in termodinamska stabilnost«).

14. Vodili smo (ali sodelovali) pri večih industrijskih projektih.

15. Sodelovali smo pri projektu z naslovom: "New carbohydrate−derived scaffolds for the generation of bioactive libraries," ki ga je finacirala Evropska komisija (5th Framework Improving Human Potential Program; HPRN-CT-2002-00173, 2004–2005).

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

The results of our research contribute toward better understanding of physico−chemical processes in living beings or/and technologically important processes. Our research focus is on nanoparticles in solutions. Some of them, e.g. proteins and DNA, are of biological importance, while others, e.g. surfactants and synthetic polyelectrolytes, are used in industrial applications. Studies of protein and DNA stability are invaluable for pharmaceutical industry and bioengineering. Wherever possible, the experimental research is complemented with theoretical analysis; the main purpose of our work is to understand these processes on the molecular level and to communicate this knowledge to students and to our colleagues in industry. During the last granting period we published 141 scientific papers in distinguished journals: Annu. Rev. Biophys. Biomol. Struc. (IF:16,2; from y. 2005 56 independent citations), Biochemistry&Molecular biol. (IF:13,3), J. Am. Chem. Soc. (IF:7,9), Nucleic Acids Res., (IF: 6.95), J. Biol. Chem. (IF: 5.8), Curr. Opin. Coll. Interface Sci. (IF:5,3), J. Phys. Chem B, J. Chem. Phys., Langmuir, Chem. Phys. Letters, and others. Three studies were published in monographic editions. Due to space limitations only a few studies are discussed below. The publications quoted are listed in the Sicris database for the period 2004–2008.

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

1. Theoretical and experimental studies of dispersed systems. Monte Carlo (MC) simulation, density functional (DFT) and integral equation theories have been used to study the structure and thermodynamic properties of model fluids in homogeneous phase and under influence of external fields [21,22,47,57,62−64,79,81,92,112,120]. Small-angle X-ray and dynamic light scattering techniques have been used to explore the structural and dynamical properties of self-assembled systems [6, 10, 52, 55], biologically relevant systems [5, 33, 43], structured solvents [71, 91] and jellifying polysaccharides [114]. We studied in−vitro release of a model drug from microemulsion [18, 52]. See also: M. Tomšič and A. Jamnik, *Simple Alcohols and their Role in Structure and Interactions of Microemulsion Systems* (Chapter 6) and M. Gašperlin and

M. Bešter Rogač, *Physicochemical Characterization of Pharmaceutically Applicable Microemulsions: Tween 40/Imwitor 308/Isopropyl Myristate/Water* (Chapter 10), V Monzer Fanun (Ed.) Microemulsions: Properties and Applications, CRC Press, Taylor & Francis, 2008. In a series of papers we studied ionic distributions between bulk solutions and charged nanoporous adsorbent [9,39,72,75,93].

2. Electrolytes and polyelectrolytes. We found divalent metal sulphates strongly hydrated even in dilute solutions; three different kinds of ionic pairs were detected [26,90,99,110]. Quint−Viallard equations [58] were used to analyze electrical conductivity of benzenehexacarboxylic acid and its acidic and neutral salts in water. We studied aqueous solutions of alkaline fulerenehexamalonates [42,87,117,119]. We measured the osmotic pressure and heats of dilution of polyanetholesulfonic acid and its alkaline salts [95]. Concentration dependence of heats of dilution of poly(L−glutaminic acid) [29] indicates the helix−coil conformational transition. Addition of polyelectrolyte to electrolyte solution enhances the reaction rate between counterions. Such catalytic effect was studied theoretically in [31,40,84,101,111]. Other theoretical studies consider the simulation of chain−like polyelectrolytes [54], interaction between spherical macro-ion and rod-like counter-ions [118] and study of influence of dielectric discontinuity on interaction between macro-ions [133]. We examined the effects of stereoregularity of poly(methacrylic acid (PMA) on its properties [11,37,73,94,143]. We showed the correlation between the stereoregularity of PMA and its thermodynamic properties.

3. Surfactant studies. We studied the interaction of surfactants with polyampholytes and oppositely charged polyelectrolytes, derivatives of fulleren and phospholipidic membranes [25,32,59,69,74,89,97]. Surfactant ion–selective membranes were used to determine the degree of binding. Micellization process of alkyltrimethylammonium chlorides with different alkyl chain length was studied by electrical conductivity [60,88,121].

4. Industrially important solutes. Salts of cyclohexylsulfamic acid, potassium acesulfame and sodium saccharin are artificial sweeteners. Total dissociation of the investigated salts in water and negligible hydration of anions [30,41,122] may influence their interaction with the receptors for taste. In dilute aqueous solutions sodium penicillin G, potassium penicillin G, and potassium penicillin V behave as acidic salts of dibasic acids, which are the final products of degradation reactions in acidic media [96].

5. Hydration of simple and complex solutes [3,128,133]. We studied the hydrophobic and ionic hydration in [8,36,76,85,86]. For this purpose we used the MC method, MD simulation and theory on the basis of the Wertheim O−Z equation. We also studied the behaviour of model water in confined systems [56]. Polyelectrolyte hydration was examined in [78]. In [107] we used MD simulation to study the influence of the counterion characteristics on its interaction with quaternary ammonium of ionen oligomer in solution.

6. Quantum chemistry and molecular similarity studies [135]. MD simulation was used to study the interaction of netropsin and DNA [20,28]. Importance of configurational changes upon netropsin and distamycin binding to the minor–groove of DNA was explored in [34]. We developed new descriptors on the basis of comparing molecular radial distribution functions (RDF) [12,61]. We collaborated in the development of GM1 mimics that could be used as a cure against cholera [65,77].

7. Biologically important molecules [134]. We contributed toward better understanding of the process of molecular recognition of DNA with small ligands [126]. We published a paper [134] that gives a most detailed review of current molecular understanding of bacterial cell death based on protein−protein and protein−DNA interactions. We managed to connect ther-

modynamics of structural transitions of intrinsically flexible (natively unfolded) protein to the bacterial cell death [19] and in another case to correlate the thermodynamics of eritropoietin unfolding with structural features of its folded and unfolded state [14]. Validity of thermodynamic models used above has been verified on less complex model processes in the micellization of surfactant molecules [60]. We have proposed a novel kinetic model that successfully describes experimentally monitored folding/unfolding transitions of some G-quadruplexes and gives positive activation energies for all elementary steps [124]. In a series of theoretical and experimental papers we studied thermodynamic and structural properties of protein−electrolyte and protein−electrolyte mixtures [43,53,83]. Experimentally we determined the solubility of lysozyme in the presence of various salts and PEG [106].

8. Crystallization. Precipitation of some industrially important solutes was studied in [1,24,94].

OTHER RELEVANT ACHIEVEMENTS

1. During this granting period we had one plenary and several keynote lectures at important international scientific conferences. We also delivered lectures at UC San Francisco, University of Coimbra, UC San Juan PR, University of Regensburg, Paul Scherrer Institute Villigen, University of Queensland, Brisbane, University Pierre and Marie Curie Paris, CEA (Saclay), Uppsala University, Institut d'Investigacions Químiques i Ambientals de Barcelona, and others.

2. From August 20–25, 2005 we organized the 29. International Conference on Solution Chemistry in Portorož. V. Vlachy acted as a chairman of the organizing committee and M. Bešter Rogač as a conference secretary. The meeting was sponsored by the International Union of Pure and Applied Chemistry. There were approx. 300 participants from 37 countries, and the Nobel laureate, Prof. Jean−Marie Lehn, was one of the lecturers.

3. V. Vlachy and M. Bešter Rogač were invited to act as guest editors of Pure and Applied Chemistry (vol. 78, 2006, no. 8.), and the Journal of Molecular Liquids (vol. 131−132, p. 1−254, 2007).

4. M. Bešter Rogač is associate editor of Acta Chimica Slovenica, and Journal of Molecular Liquids (Elsevier).

5. V. Vlachy was elected a member of Academia Scientarum et Artium Europaea.

6. A. Godec, SZF award: Prometheus in Science Award for excellence in communication in 2008.

7. Members of the group were mentors to students whose works were granted the F. Prešeren Awards at the University or Faculty level, and the Krka Awards.

8. In last four years several members of the group made three, or more month visits to foreign universities (Jožica Dolenc – ETH Zurich, Alan Bizjak – UC San Francisco, Miha Lukšič – University of Regensburg, Matjaž Bončina – Max–Planck Institut für Polymerforschung, Mainz).

9. In 2006/07 V. Vlachy was acting as a Visiting Professor at UC San Francisco, six months at University of Regensburg, and one month at Université Pierre et Marie Curie, Paris–6, France.

10. V. Vlachy was elected to serve as "Adjunct Professor" at the Department of Pharmaceutical Chemistry, University of California San Francisco.

11. We have a continuous collaboration via bilateral projects with Austria, Hungary, Croatia, Portugal, USA, France, and Ukraine.

12. For the last eight years we have been cooperating with partners from the UC San Francisco in the project entitled "Solvation in Biology" financed by the National Institute of Health.

13. We participate in two COST projects (D–31 G. Vesnaver, D–43 M. Bešter Rogač), and have one postdoctoral project (J. Dolenc, Molecular dynamics simulation of nucleic acids: structure, dynamics and thermodynamic stability).

14. We have been principal investigators or co-investigators in several industrial projects.

15. We participated in the "New carbohydrate–derived scaffolds for the generation of bioactive libraries" programme, which was funded by the European Commission's 5th Framework Improving Human Potential Program. HPRN-CT-2002-00173 (2004–2005).

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

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POROČILO O REALIZACIJI PROGRAMA

CILJI PROGRAMA

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

Program se je tesno prepletal z več multilateralnimi in bilateralnimi mednarodnimi programi (EU, ostale države v Evropi in ZDA), kot tudi z raziskovalnimi programi več domačih akademskih (UL Medicinska fakulteta, UL Fakulteta za farmacijo, Narodna in univerzitetna knjižnica, Kemijski inštitut) in industrijskih raziskovalnih ustanov (Krka, Lek). Naše raziskovalno delo je bilo usmerjeno v načrtovanje novih sinteznih metod, reagentov in reakcij, ki bi omogočile sintezo spojin s ciljnimi biološkimi aktivnostmi. Del naših raziskav se je odvijal tudi v okviru raziskovalnega projekta *Od multifunkcionalnih gradnikov do biološko aktivnih spojin (J1-6693-0103)*. Drugi del raziskav je bila organska sinteza kot del Petega okvirnega programa (*InkCor, EVKA4-CT-2001-00049*, koordinatorica J. Kolar). Dva naša raziskovalca (B. Štefane in F. Požgan) sta v tem obdobju (2004–2008) zaključila s post-doktorskim izobraževanjem v okviru EU *Marie Curie* štipendijskega programa.

OSREDNJE TEME PROGRAMA IN ZNANSTVENI DOSEŽKI

Na področju cikličnih aminokislinskih derivatov smo raziskali Diels−Alderjevo reakcijo 2*H*-piran-2-onov z alkini, pri kateri so nastali visoko substituirani derivati anilina, kot npr. *orto*-fenilendiamini. Usmerili smo se tudi v raziskave pretvorb 3-benzoilamino-6-metil-2*H*-piran-2-onov, ki so na položaju 5 vsebovali elektron-akceptorsko skupino (K. Kranjc, B. Štefane, S. Polanc, M. Kočevar, *J. Org. Chem.* 2004, *69*, 3190) ali elektron-donorsko skupino (K. Kranjc, M. Kočevar, *New J. Chem.* 2005, *29*, 1027), z elektronsko bogatimi kot tudi z elektronsko osiromašenimi alkini. Raziskane pretvorbe so pomembne s stališča sinteze, saj omogočajo pripravo množice različnih polisubstituiranih anilinskih, bifenilnih in terfenilnih derivatov. Reakcije smo raziskali pod termičnimi pogoji in pod visokimi tlaki (12 kbar). Pokazali smo, da je možno vplive substituentov na reaktivnost in regioselektivnost razložiti s pomočjo elektronskih zahtev reakcij, ki potekajo preko polariziranih asinhronih koncertiranih prehodnih stanj ali pa preko zwitterionskih intermediatov. Teh zadnjih reakcijskih intermediatov sicer nismo zaznali, vendar lahko vseeno nekatere pretvorbe s pomočjo obstoja zwitterionov razložimo bolj učinkovito, kot če upoštevamo potek preko prehodnega stanja. Pomembno je tudi poudariti, da je zwitterion v bistvu skrajni primer prehodnega stanja. Z našimi raziskavami smo tudi dokazali, da so reakcije pod visokimi tlaki vodene z drugače izraženimi vplivi kot pri običajnem tlaku. Po drugi strani pa je z DABCOm katalizirana cikloadicija etil vinil etra na 2*H*-piran-2-one pokazala, da se lahko etil vinil eter uspešno uporabi kot sintezni ekvivalent za acetilen v pripravi serije derivatov anilina (K. Kranjc, M. Kočevar, *Synlett* 2008, 2613). Praktično uporabnost 2*H*-piran-2-onov smo pokazali z dvostopenjsko pretvorbo v indole. V prvi stopnji so z Diels−Alderjevo cikloadicijsko reakcijo (*Z*)-1-metoksibut-1-en-3-ina in 5,6-disubstituiranih 3-acilamino-2*H*-piran-2-onov pod pogoji obsevanja z mikrovalovi, s klasičnim segrevanjem ali pa pod visokimi tlaki (13−15 kbar) nastali ustrezni benzenski derivati z 2-metoksietenilno skupino na ključnem položaju. Tako pripravljeni adukti so pod rahlo kislimi pogoji zlahka ciklizirali v 1,5,6-trisubstituirane indolne derivate (K. Kranjc, M. Kočevar, *Tetrahedron* 2008, *64*, 45).

Ugotovili smo tudi, da je Diels−Alderjevo reakcijo *2H*-piran-2-onov s serijo *N*-substituiranih maleimidov, pri kateri nastanejo pripojeni biciklo[2.2.2]okteni, možno izvajati v vodnih raztopinah pod pogoji obsevanja z mikrovalovi. Kadar so občutljive funkcionalne skupine del izhodnih spojin, se je izkazalo za bolj učinkovito izvajanje teh reakcij brez dodatka topila (K. Kranjc, M. Kočevar, *Heterocycles* 2007, *73*, 481). Podoben tip produktov smo pripravili iz različno substituiranih 2,3;5,6-dianhidridov biciklo[2.2.2]okt-7-en-2*ekso*,3*ekso*,5*ekso*,6*ekso*-tetrakarboksilnih kislin in seta hidrazinov. V vodnih raztopinah so ob obsevanju z mikrovalovi z visokimi izkoristki nastali ustrezni pripojeni *N*-aminosukcinimidi. Kadar je izhodna spojina vsebovala dodatno acetilno skupino, je reagirala tudi ta, pri čemer so kot edini produkti nastali ustrezni hidrazonski derivati *N*-aminosukcinimidov (J. Hren, K. Kranjc, S. Polanc, M. Kočevar, *Heterocycles* 2007, *72*, 399).

2*H*-Piran-2-oni so se izkazali tudi kot zelo učinkoviti sintoni za pretvorbe v različne heterociklične sisteme. Še posebno podrobno smo raziskali pretvorbe v derivate piridazina, ki smo jih nadalje uporabili kot substrate za pripravo serije heterocikličnih spojin, zlasti učinkovito kadar smo kot oksidant uporabljali amonijev cerijev(IV) nitrat (CAN). Tu smo celo uspeli izolirati intermediat in s tem omogočili razjasnitev celotne pretvorbe (F. Požgan, S. Polanc, M. Kočevar, *Tetrahedron* 2006, *62*, 9718; F. Požgan, S. Kafka, S. Polanc, M. Kočevar, *Heterocycles* 2006, *70*, 235). Raziskovali smo tudi migracijo 2*H*-piran-2-onske enote pod pogoji Schmidtove reakcije ter zaznali prvo migracijo te skupine v zgoraj opisani reakciji (F. Požgan, M. Krejan, S. Polanc, M. Kočevar, *Heterocycles* 2006, *69*, 123).

Iz ustreznih alkanonov, *N*,*N*-dimetilformamid dimetil acetala (DMFDMA) in hipurne kisline v prisotnosti velikih prebitkov acetanhidrida smo sintetizirali tudi serijo 3-benzoilnih derivatov 5- do 8-členskih cikloalka[*b*]piran-2-onov ter 2*H*-piran-2-onov z uporabo že opisanih metod (F. Požgan, K. Kranjc, V. Kepe, S. Polanc, M. Kočevar, *ARKIVOC* 2007, (*viii*), 97).

Raziskali smo tudi reaktivnost nekaterih enostavnih α-aminokislinskih derivatov (derivatov oksazol-5(4*H*)-onov, 2-aminopropenojske kisline in diaminomaleonitrila) ter njihovo uporabnost pri sintezah nekaterih analogov naravnih produktov ter ostalih heterocikličnih spojin. Iz diaminomaleonitrila, 4-etoksimetilen-2-fenil-5(4*H*)-oksazolona in alkil ali cikloalkil alkoholov smo razvili dve enostavni metodi priprave substituiranih 2-amino-3-(vinilamino)propenoatov (T. Trček, B. Verček, *Acta Chim. Slov*. 2005, *52*, 171). Razvili smo tudi novo metodo sinteze serije alkil 3-(imidazol-1-il)propenoatov iz *N*-oksazolidenmetil substituiranih diaminomaleonitrilov (T. Trček, B. Verček, *ARKIVOC* 2005, (*xiv*), 96). Raziskali smo tudi štiri *one-pot* postopke priprave visoko funkcionaliziranih imidazo[1,5-*a*]pirazinov, ki temeljijo na pretvorbi dveh derivatov diaminomaleonitrila ter dveh imidazolskih derivatov (T. Trček, B. Verček, *Synthesis* 2006, 3437). Nekatere benzoilaminometil substituirane triazoloazine smo pripravili z reakcijo med acilglicini in heteroarilhidrazini (I. Mušič, B. Verček, *Heterocycl. Commun*. 2005, *11*, 321). Opisali smo tudi enostavno sintezno metodo priprave serije 1,4-disubstituiranih-5-hidroksi-1*H*-pirazolov iz 4-hidroksimetiliden-2-feniloksazol-5(4*H*)-onov in različnih fenilhidrazinov, ki poteka preko etil 2-(benzoilamino)-3-(fenilhidrazono)propanoatov (K. Čuček, A. Golobič, B. Verček, *Heterocycles* 2007, *73*, 555). Dodatno smo s segrevanjem etil 2-(benzoilamino)-3-(fenilhidrazono)propanoatov ob prisotnosti polifosforne kisline pripravili številne etil 3-(benzoilamino)-1*H*-indol-2-karboksilate (K. Čuček, B. Verček, *Synthesis* 2008, 1741).

Udeleženi smo bili tudi v okviru EU programa COST D24/007/02, ki je bil sestavljen iz 8 raziskovalnih skupin in katerega cilj je bil razvoj novih katalitskih in selektivnih metod (zlasti hidrogeniranj in oksidacij) pod pogoji heterogene katalize. Naša vloga v tem programu je bila razvijanje industrijsko pomembnih substratov (α,β-didehidro-α-aminokislinskih derivatov in nenasičenih karbonilnih spojin), ki jih s klasičnimi metodami ne bi bilo mogoče

pretvarjati naprej, mi pa bi jih uporabili za prilagajanje novorazvitih tehnik enantioselektivnih redukcij ter oksidacij. V tem programu smo raziskali tudi pripravo koloidov platine, modificiranih s kiralnim ligandom sinfos, s ciljem priprave katalitskih nanomaterialov. Koloide smo nato vključili v silicijev dioksid ter tako pripravili heterogene katalizatorje. Te koloide, tako »kvazi-homogene katalizatorje« (oz. topne heterogene katalizatorje) kot tudi vključene v silicijev dioksid (heterogene katalizatorje), smo uporabili pri selektivni hidrogenolizi sterično močno napetih biciklo[2.2.2]okt-7-enov in pri hidrogeniranju etil piruvata. Želimo poudariti, da naša metodologija odpira nove aspekte kemije biciklo[2.2.2]oktenov, saj namesto pričakovanega hidrogeniranja dvojne vezi poteče njena cepitev, pri čemer nastanejo visoko substituirani multifunkcionalni cikloheksanski gradniki (F. Neațu, A. Kraynov, V. I. Pârvulescu, K. Kranjc, M. Kočevar, V. Ratovelomanana-Vidal, R. Richards, *Nanotechnology* 2008, *19*, art. no. 225702 (8 pp)). Drugi katalizator za selektivno hidrogenolizo gornjih substratov smo pripravili iz Fe_3O_4 koloidov, modificiranih s kiralnim ligandom cinkonidinom in končno vključenim v silicijev dioksid (F. Neațu, A. Kraynov, L. D'Souza, V. I. Pârvulescu, K. Kranjc, M. Kočevar, V. Kuncser, R. Richards, *Appl. catal., A Gen.* 2008, *346*, 28).

Objavili smo tudi pregledni članek o sintezi in pretvorbah pripojenih biciklo[2.2.2]oktenov (J. Hren, S. Polanc, M. Kočevar, *ARKIVOC* 2008, (*i*), 209).

Organski BF_2 kelati so se izkazali kot zanimivi intermediati v organskih pretvorbah. Pripravili smo nekatere BF_2 kelate ter raziskali njihove pretvorbe. Odkrili smo doslej še neznano neposredno pretvorbo 5,6-disubstituiranih 2,2-difluoro-4-alkoksi-1,3,2-dioksaborinanov z različnimi amini v 2,2-difluoro-4-alkilamino analoge. Prikazali smo tudi preparativno uporabno metodo za sintezo β-keto amidov in β-enamino karboksamidov v dveh stopnjah in z dobrimi izkoristki, izhajajoč iz lahko dostopnih začetnih spojin. Ta kemo- in regioselektivni pristop bi bil lahko izbrana metoda za pripravo tovrstnih sistemov (B. Štefane, S. Polanc, *Synlett* 2004, 698; *Tetrahedron* 2007, *63*, 10902).

Oksidacija aril in heteroarilhidrazinov ter hidrazidov s CAN vodi do različnih produktov. Potek reakcije je močno odvisen od narave substrata. V večini primerov smo kot končne produkte izolirali ogljikovodike ali alkoksi derivate. Kadar smo uporabljali devterirana topila, kot npr. metanol-d_4 ali acetonitril-d_3, smo dosegli regiospecifično vključitev devterija (B. Štefane, S. Polanc, *Synlett* 2008, 1279).

Študije kemije diazenov so pokazale, da dialkil diazendikarboksilati reagirajo s 4-fluorofenolom ob prisotnosti $ZrCl_4$, pri čemer nastanejo derivati 2-klorofenola, aminirani na položaju 4 glede na OH skupino (S. Bombek, F. Požgan, M. Kočevar, S. Polanc, *J. Org. Chem.* 2004, *69*, 2224). Reakcije metil cikloheksilaminokarbonildiazendikarboksilata in metil (2-kloroetilamino)karbonildiazenkarboksilata z 1,3-diketoni, β-keto estri ter β-keto amidi v prisotnosti natrijevega acetata vodijo do ustreznih Michaelovih aduktov kot stabilnih produktov. Te smo obdelali z ionskim izmenjevalcem (Dowex) in tako pripravili substituirane 2-imidazolin-2-one. Vpliv baze je bistven za rezultat reakcije. Ob prisotnosti DBN so Michaelovi adukti reagirali še naprej; ciklizirali so namreč v 2-imidazolidinone, ki smo jih z Dowexom kvantitativno pretvorili v 2-imidazolin-2-one kot končne produkte. *N*-Fenilacetoacetamid reagira z zgoraj omenjenimi diazeni ob prisotnosti DBN, pri čemer nastane zmes dveh produktov, ki smo ju ločeno obdelali s CF_3CO_2D ter z NMR zasledovali eliminacijo vode. Uporaba β-keto amidov, še posebej acetoacetamida in *N*-fenilacetoacetamida, za pripravo imidazolonov je pomembna zaradi naraščajočega zanimanja za biološko aktivne amide imidazolkarboksilnih kislin (S. Bombek, F. Požgan, M. Kočevar, S. Polanc, *New J. Chem.* 2005, *29*, 948). Pred kratkim smo opisali prvi primer uporabe zmesi $ZrBr_4$ in diazena za selektivno bromiranje različnih fenolov, aromatskih etrov in anilinov. Metoda je popolnoma regioselektivna in s tem omogoča

mnoge sintezne uporabe. Reakcija poteka pod milimi pogoji, atom broma se najprej veže na *para* nesubstituiran položaj glede na OH, OR ali NR_2 skupine ustrezno aktiviranih aromatskih substratov. Manj reaktivne spojine, kot npr. toluen, fenil acetat, benzonitril in trifluorometilbenzen, ostanejo pod temi pogoji nezreagirane. Mili reakcijski pogoji, relativno hitra pretvorba, dobri do odlični izkoristki in selektivnost so glavne odlike tega postopka (T. Stropnik, S. Bombek, M. Kočevar, S. Polanc, *Tetrahedron Lett.* 2008, *49*, 1729).

Ovrednotili smo tudi potencial tetrametilamonijevega klorida kot alternativnega reagenta za metiliranje fenolov pod mikrovalovnimi pogoji. Ugotovili smo, da se da mnoge enostavne fenole metilirati v prisotnosti K_2CO_3, medtem ko nekateri drugi manj reaktivni fenoli zahtevajo prisotnost bolj reaktivnega Cs_2CO_3 (N. Maraš, S. Polanc, M. Kočevar, *Tetrahedron* 2008, *64*, 11618).

Študije 1,3-diariltriazenov so pokazale, da trietilamonijevi triazenidi že pri sobni temperaturi reagirajo z alkil propiolati, pri čemer z visokimi izkoristki nastanejo alkoksikarbonilviniltrietilamonijevi triazenidi. Enake spojine smo izolirali tudi, če smo v zmes alkil propiolata in izbranega triazena v acetonitrilu dodali trietilamin. Izkazalo se je, da z alkoksikarbonilviniltrietilamonijevimi triazenidi potekajo transesterifikacije. V tem procesu igra bistveno vlogo triazenid kot protiion (A. Virag, A. Meden, M. Kočevar, S. Polanc, *J. Org. Chem.* 2006, *71*, 4014).

V sodelovanju z raziskovalno skupino dr. M. Osmak (Inštitut Ruđer Bošković, Zagreb) smo raziskali citotoksičnost več spojin. Zelo dobre rezultate smo dobili z *N*-(2-kloroetil)-2-(2,3,4,5,6-pentafluorofenil)diazenkarboksamidom. IC_{50} za to spojino je za različne rakaste celice v območju 16−42 μM. Vredno je tudi omeniti, da ta spojina ne inhibira le rasti matičnih celic, marveč tudi rast celic, odpornih na nekatere učinkovine, npr. cisplatin, vinkristin in doksorubicin (T. Čimbora-Zovko, S. Bombek, J. Košmrlj, L. Kovačič, S. Polanc, A. Katalinić, M. Osmak, *Drug Develop. Res.* 2004, *61*, 95). Dejstvo, da ti diazeni tudi selektivno oksidirajo tiole v disulfide, se kaže tudi v njihovem vplivu na znotrajcelično raven glutationa. Dodatno mnogi diazeni kažejo tudi močno citotoksičnost proti različnim človeškim matičnim tumornim celicam ter tudi proti njihovim podlinijam, sicer odpornim na nekatere učinkovine (S. Polanc, *J. Heterocycl. Chem.* 2005, *42*, 401). Pregled biološke aktivnosti diazenov je tudi pokazal, da nekatere strukturno podobne spojine kažejo bistveno različne citotoksičnosti, kar se zdi, da je povezano z razliko v bazičnosti določenih fragmentov teh molekul (S. Jakopec, K. Dubravčić, A. Brozović, S. Polanc, M. Osmak, *Cell Biology and Toxicology* 2006, *22*, 61). *N*-Fenil-2-(2-piridinil)diazenkarboksamid pa povzroča »apoptozi podobno« vrsto programirane celične smrti rakastih celic maternič-nega vratu (S. Jakopec, K. Dubravčić, S. Polanc, J. Košmrlj, M. Osmak, *Toxicology in Vitro* 2006, *20*, 217). Serijo 16 diazenov smo tudi testirali na štirih linijah človeških levkemičnih celic (NALM-1, JURKAT, HL-60 in K-562). Enajst izmed teh diazenov je bilo citotoksičnih proti levkemičnim celicam, vendar pa niso učinkovali na normalne človeške monojedrne krvne periferne celice v fazi mirovanja. Osem diazenov pa ni vplivalo niti na normalne celice v dobi delitve niti na Con-A stimulirane PBMC in 3T3 fibroblaste. Opažena selektivna citotokstičnost diazenov torej obeta njihovo možno uporabo kot spojin pri zdravljenju pacientov z levkemijo (I. Martin-Kleiner, S. Bombek, J. Košmrlj, B. Čupić, T. Čimbora-Zovko, S. Jakopec, S. Polanc, M. Osmak, J. Gabrilovac, *Toxicology in Vitro* 2007, *21*, 1453).

D-Alanin-D-alanin ligaza (Ddl) katalizira biosintezo D-alanil-D-alanina, ki je esencialni bakterijski prekurzor peptidoglikana ter s tem predstavlja pomembno tarčo za razvoj novih antibakterijskih zdravil. Sledeč temu cilju, smo pripravili serijo diazendikarboksamidov ter študirali njihovo inhibitorno aktivnost na DdlB iz *E. coli*. Trinajst spojin je bilo boljših inhibitorjev od D-cikloserina, pet izmed njih pa je imelo IC_{50} vrednosti pod 50 μM. Ti inhibitorji so strukturno drugačni od ADP in tudi od D-alanina, zato pričakujemo, da Ddl inhibirajo z novim načinom vezave. Ker imajo mnogi diazendikarboksamidi tudi antimikrobno aktivnost

in vitro, predstavljajo obetaven začetek za nadaljnje raziskave. Zgoraj navedene študije smo izvedli v sodelovanju s prof. S. Gobcem s Fakultete za farmacijo Univerze v Ljubljani in prof. I. Chopro z Univerze Leeds, Velika Britanija (A. Kovač, V. Majce, R. Lenaršič, S. Bombek, J. M. Bostock, I. Chopra, S. Polanc, S. Gobec, *Bioorg. Med. Chem. Lett.* 2007, *17*, 2047; patentna prijava: S. Gobec, A. Kovač, A. Brajić, S. Pečar, J. Bostock, I. Chopra, R. Lenaršič, S. Bombek, M. Kočevar, S. Polanc, *Diazenedicarboxamides as inhibitors of D-alanine: D-alanine ligaes (Ddl) : European patent no. EP07468010, publication date: 07. avgust 2007*. Munich: European Patent Organisation, 2007.).

Povezava dveh aktivnih molekul z mostom, ki ga je enostavno razcepiti, predstavlja nov tip potencialno aktivnih molekul, ki smo jih raziskovali v sodelovanju s prof. J. Vinšovo s Fakultete za farmacijo Karlove univerze, Hradec Králové. Sinteza temelji na derivatih, izvirajočih iz izonikotinoil hidrazida (INH), pirazinamida (PZA), *para*-aminosalicilne kisline, etambutola in ciprofloksacina. Raziskovali smo lipofilno, hidrolitično (stabilnost spojin) in antituberkulozno aktivnost, kot tudi odnos med strukturo in lipofilnostjo ter strukturo in aktivnostjo. Ugotovili smo, da je hitrost hidrolize novih produktov odvisna od fragmentov teh molekul. Antituberkulozno aktivnost smo ugotavljali proti *M. tuberculosis H37Rv* in proti trem netuberkuloznim sevom. Tri nove spojine so imele večjo aktivnost proti netuberkuloznim sevom kot INH in PZA, ki sta bila uporabljena kot interna standarda. Kot dodatna prednost se izkaže, da hidroliza novih spojin zagotavlja podaljšano sproščanje aktivnih komponent (A. Imramovský, S. Polanc, J. Vinšová, M. Kočevar, J. Jampílek, Z. Rečková, J. Kaustová, *Bioorg. Med. Chem.* 2007, *15*, 2551).

V sodelovanju z raziskovalno skupino prof. dr. S. Kafke in prof. dr. A. Kláska (Univerza Tomas Bata, Zlin, Češka republika; bilateralni projekti: BI-CZ/03-04-5, BI-CZ/05-06/009, BI-CZ/07-08-018) smo nadaljevali z raziskavami kinolin-2,4(1*H*,2*H*)-dionov na področju ustreznih 3-hidroksi, 3-tio in 3-amino analogov, kot je opisano spodaj.

Ugotovili smo, da se nekateri 3-hidroksikinolin-2,4(1*H*,3*H*)-dioni v bazičnih vodnih medijih premestijo v strukturno raznovrstne produkte. Tako je 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 spremljal nastanek dveh stranskih produktov s spiro[2*H*-indol]-3(1*H*)-onskima skeletoma. Strukture teh spojin smo določili z NMR in MS ter potrdili z rentgensko difrakcijo. Strukturna analiza spiro[2*H*-indol]-3(1*H*)-onov je pomembna, saj je ta motiv moč najti v nekaterih naravnih produktih in tudi kot ključni del nekaterih biološko aktivnih molekul ter spojin s fotokromnimi lastnostmi (J. Košmrlj, S. Kafka, I. Leban, M. Grad, *Magn. Reson. Chem.* 2007, *45*, 700).

Raziskovali smo tudi reaktivnost derivatov v katerih je 3-hidroksi skupina zaščitena v obliki estra. V tej smeri smo 3-hidroksikinolin-2,4(1*H*,3*H*)-dione z Wittigovo olefinacijo z etil (trifenilfosforaniliden)acetatom ($Ph_3P{=}CHCO_2Et$) pretvorili v furo[2,3-*c*]kinolin-2,4(3a*H*,5*H*)-dione, ki so se pod termičnimi pogoji z bazično katalizirano reakcijo premestili v furo[3,4-*c*]kinolin-3,4(1*H*,5*H*)-dione. Predlagali smo mehanizem te premestitve, rezultate pa smo objavili v obliki predhodne komunikacije (S. Kafka, J. Košmrlj, A. Klásek, A. Pevec, *Tetrahedron Lett.* 2008, *49*, 90).

V povezavi s 3-tio analogi smo raziskali novo tandemsko hidratacijo α-tiocianatoketonov v tiokarbamate, ki ji je sledila in situ ciklodehidratacija v prikondenzirane 2-okso-2-tiazoline. To reakcijo smo uporabili pri sintezi [1,3]tiazolo[5,4-*c*]kinolin-2,4(3a*H*,5*H*)-dionov iz 3-tiocianatokinolin-2,4(3a*H*,5*H*)-dionov. Ker v literaturi obstaja le majhno število strategij za pripravo prikondenziranih 2-okso-3-tiazolinov, predstavlja naš prispevek pomembno novo metodo. Želimo tudi poudariti, da so te strukture pomembne, saj imajo podobni 2-ariltiazolo[4,5-*c*]kinolin-4(5*H*)-oni veliko afiniteto za GABA receptor (A. Klásek, V. Mrkvička, A. Pevec, J. Košmrlj, *J. Org. Chem.* 2004, *69*, 5646).

Na področju 3-aminoanalogov, smo izbrane 3-aminokinolin-2,4(1*H*,3*H*)-dione pretvorili v pirolo[2,3-*c*]kinolin-2,4(3a*H*,5*H*)-dione. Za ta namen smo raziskali dva alternativna pristopa; inter- in intramolekularno Wittigovo olefinacijo. Začetni poizkusi so potrdili, da pirolo[2,3-*c*]kinolin-2,4(3a*H*,5*H*)-dioni pod bazičnimi pogoji izomerizirajo v ustrezne pirolo[3,4-*c*]kinolin-3,4(2*H*,5*H*)-dione. Še nobeden od teh skeletov predhodno ni bil opisan v literaturi (S. Kafka, A. Klásek, J. Polis, V. Rosenbreierová, C. Palík, V. Mrkvička, J. Košmrlj, *Tetrahedron* 2008, *64*, 4387).

Medtem ko pri segrevanju *S*-(3-alkil/aril-2,4-diokso-1,2,3,4-tetrahidrokinolin-3-il)tiokarbamatov nastanejo 4-hidroksi-1*H*-kinolin-2-oni, pod enakimi reakcijskimi pogoji 3a-alkil/aril-[1,3]tiazolo[5,4-*c*]kinolin-2,4(3a*H*,5*H*)-dioni, odvisno od substituenta na obročnem dušiku, reagirajo v dva različna tipa produktov. Alkil ali aril substituirani substrati reagirajo v 4-amino-3-alkil/aril-1*H*-kinolin-2-one, medtem ko se na dušiku nesubstituirani analogi premestijo v nove 6*H*-tiazolo[3,4-*c*]kinazolin-3,5-dione. Študirali smo mehanizem omenjenih transformacij (V. Mrkvička, A. Klásek, R. Kimmel, A. Pevec, J. Košmrlj, *ARKIVOC* 2008, (*xiv*), 289).

Dosegli smo prve rezultate v zvezi s predlogom programa P1-0230 Organska kemija: sinteza, struktura in aplikacija (2009-13), kot sledi. Azomide, ki so se v naših predhodnih študijah izkazali kot bioaktivni agenti za redukcijo intracelularnega glutationa (GSH), smo opremili s terminalno alkinsko (propargilno) skupino. Tako nastale propargil-funkcionalizirane azoamide smo nato s cikloadicijo z azidi, katalizirano z bakrom(I), pretvorili v različne azoamide, funkcionalizirane z ligandnimi ročicami. V tej študiji smo uporabili azide, ki so imeli ligandne ročice, za katere je znano, da se lahko vežejo na platino(II). Za cikloadicije med azidi in relativno krhkimi propargil-funkcionaliziranimi azoamidi smo testirali različna topila in bakrove katalizatorje. Tipični reakcijski pogoji, ki so pogosto uporabljeni za zgoraj omenjeno cikloadicijo, namreč niso bili primerni. Odlične rezultate smo dobili z uporabo kombinacije bakrovega(II) sulfata pentahidrata in kovinskega bakra, še posebej pa z uporabo heterogenih katalizatorjev: bakra na oglju, bakrovega(I) oksida in bakrovega(II) oksida. Z uporabo teh heterogenih katalizatorjev smo produkte cikloadicije (z ligandnimi ročicami funkcionalizirane azoamide) dobili s skoraj kvantitativnimi izkoristki v enostavnem tri-stopenjskem procesu ‘mešanje-filtracija-uparevanje’. Z uporabo heterogenih katalizatorjev produkti niso bili kontaminirani z bakrom, kar je posebej pomembno, saj so produkti načrtovani za koordinacijo na kovinske ione. Ta raziskava prikazuje modularen pristop, ki omogoča pripravo različnih, z ligandnimi ročicami funkcionaliziranih, azoamidov. Le-te bomo preučili kot potencialne bioaktivne ligande v novih cisplatin analogih, hibridnih molekulah z dvojnim načinom delovanja v zdravljenju raka. Poleg tega bodo rezultati predstavljeni v tem delu našli aplikacije v avtomatizirani »klik« kemiji (D. Urankar, J. Košmrlj, *J. Comb. Chem.* 2008, *10*, 981).

Etilidenmalononitrilno stransko verigo v {1-[6-(dimetilamino)-2-naftil]etiliden}malononitrilu (DDNP) smo z dvostopenjskim procesom pretvorili v substituirane piridinske obroče. V reakciji nitrilne skupine s HCl v alkoholnih raztopinah smo ujeli kloroimidatni intermediat v obliki 2-kloro-4-[6-(dimetilamino)-2-naftil]nikotinonitrila, kar dokazuje njegov obstoj pri Pinnerjevi sintezi. Hkrati smo ga z nukleofilno zamenjavo klora izkoristili kot začetno spojino za pripravo več derivatov. Strukturo 2-metilaminskega derivata smo tudi dokazali z rentgensko analizo (P. Škofic, C. Dambrot, M. Koželj, A. Golobič, J. R. Barrio, A. Petrič, *Acta Chim. Slov.* 2005, *52*, 391).

V sodelovanju z raziskovalci z Medicinske fakultete UL smo pokazali, da markiranje s FDDNP zanesljivo napoveduje dvolomnost v točno določenih mikroskopskih strukturah histoloških preparatov, obarvanih s Kongo rdečim, pri klasičnih boleznih, povzročenih z amiloidnimi nanosi, kot so npr. Alzheimerjeva bolezen, cerebralna amiloidna angiopatija ter nalezljive

spongiformne encelopatije (A. Šmid, T. D. Vovko, M. Popović, A. Petrič, V. Kepe, J. R. Barrio, G. Vidmar, M. Bresjanac, *Brain Pathol.* 2006, *16*, 124). Zaradi izjemnega zanimanja za uporabo 2-(1-{6-[(2-[^{18}F]fluoroetil)(metil)amino]-2-naftil}etiliden)malononitrila ([^{18}F]FDDNP) v PET (pozitronska emisijska tomografija) raziskavah nevrodegenerativnih okvar, pri katerih se v centralnem živčnem sistemu nalagajo proteinski agregati, smo razvili avtomatizirano radiosintezo, ki daje produkt z visokim izkoristkom. Metoda je hitra, zanesljiva in primerna za pripravo velikih množin (>150 mCi) [^{18}F]FDDNP za študije pri glodalcih in ljudeh (J. Liu, V. Kepe, A. Žabjek, A. Petrič, H. C. Padgett, N. Satyamurthy, J. R. Barrio, *Mol. Imaging Biol.* 2007, *9*, 6).

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

DRUGI RELEVANTNI DOSEŽKI

Cilj raziskovalnega projekta *Od multifunkcionalnih gradnikov do biološko aktivnih spojin (J1-6693-0103)* je bil razvijanje sintez in nadaljnje preoblikovanje različno substituiranih multifunkcionalnih gradnikov, ki bi jih bilo mogoče uporabiti kot modelne spojine za razvijanje novih metod na področju organske kemije (selektivne sinteze), kakor tudi priprava spojin s potencialno biološko aktivnostjo, ki bi jih lahko vgradili v bolj kompleksne spojine. Raziskovalni program je predstavljal del aktivnosti v mednarodnem programu EU COST D24 Action Sustainable Chemical Processes: Stereoselective Transition Metal-Catalysed Reactions (D24/0007/02: Synthesis and Application of New Ligands for Asymmetric Heterogeneous Catalysis).

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PLENARNA IN VABLJENA PREDAVANJA

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

DRUGE DEJAVNOSTI

M. Kočevar je Nacionalni predstavnik v odboru (komiteju) Organic and Biomolecular Chemistry Division (III) IUPAC (za obdobje 2008−2009) in član upravnega odbora COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011). *Uredniško delo:* J. Košmrlj je bil v letih 2003−2005 glavni in odgovorni urednik *Acta Chimica Slovenica* (ACS), K. Kranjc je član uredniškega sveta ACS (2007−), M. Kočevar pa član uredniškega odbora *Periodica polytechnica. Chemical engineering* (2003−), bil pa je tudi član uredniškega odbora za *Slovenski veliki leksikon*. S. Polanc je član uredniškega odbora *Topics in heterocyclic chemistry* (2008−).

NAGRADE

A. Petrič in J. Košmrlj sta (skupaj z A. Pavkom) prejela nagrado Maksa Samca za popularizacijo študijev na FKKT UL.

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

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

The programme is tightly intertwined with several multilateral and bilateral international programs (EU, other European countries and USA), as well as with the research programs at several academic institutions in Slovenia (UL Faculty of Medicine, UL Faculty of Pharmacy, National and University Library, National Institute of Chemistry) and industrial research institutions (Krka, Lek). Our research efforts were directed at developing new synthetic methods, reagents, and reactions to provide access to compounds which possess targeted biological activities. Part of our investigations took place within the research project *From multifunctional building blocks to biologically active compounds (J1-6693-0103)*. Another part of our investigation was also the organic synthesis research, incorporated in the 5th Framework project (*InkCor, EVKA4-CT-2001-00049*, coordinator J. Kolar). Two of our researchers (B. Štefane and F. Požgan) finished their postdoctoral training within the framework of the EU *Marie Curie Grant* postdoctoral fellowship program during the period 2004−2008.

RESEARCH TOPICS AND SCIENTIFIC ACHIEVEMENTS

In the field of cyclic amino acid derivatives research we investigated the Diels−Alder reaction of 2*H*-pyran-2-ones with alkynes, in which highly substituted derivatives of aniline, such as *ortho*-phenylendiamine were obtained. We focused our attention on the transformations of 3-benzoylamino-6-methyl-2*H*-pyran-2-ones containing an electron withdrawing group at the position 5 (K. Kranjc, B. Štefane, S. Polanc, M. Kočevar, *J. Org. Chem.* 2004, *69*, 3190) or an electron donating group (K. Kranjc, M. Kočevar, *New J. Chem.* 2005, *29*, 1027), with alkynes containing both electron donating or electron withdrawing groups in their structures. The transformations investigated are important from the synthetic point of view, because they yield a variety of polysubstituted aniline, biphenyl and terphenyl drivatives. We have investigated reactions under thermal conditions and under high pressure (12 kbar). It was shown that the effect of substituents on the reactivity and regioselectivity can be explained in terms of electron demands *via* polarized asynchronous concerted transition state or by the formation of a zwitterionic intermediate. The latter has not been detected as the reaction intermediate; nevertheless, some transformations can be more efficiently explained taking into account its existence instead of the transition state. It is also important to mention that the zwitterion is, in fact, the extreme case of the transition state. During our investigations we have also proven that the reactions under high pressures are governed by differently pronounced factors than those at normal pressure. On the other hand, the DABCO-catalyzed cycloaddition of ethyl vinyl ether onto 2*H*-pyran-2-ones has shown that ethyl vinyl ether can be successfully used as a synthetic equivalent of acetylene in the preparation of a series of aniline derivatives (K. Kranjc, M. Kočevar, *Synlett* 2008, 2613). A practical application of 2*H*-pyran-2-ones was demonstrated in their two-step transformation to indoles. In the first step, the Diels−Alder cycloaddition reaction of (*Z*)-1-methoxybut-1-en-3-yne with 5,6-disubstituted 3-acylamino-2*H*-pyran-2-ones under microwave irradiation conditions, with classical heating or at high-pressures (13−15 kbar) yields the corresponding benzene derivatives with a strategically positioned 2-methoxyethenyl moiety. The adducts thus

prepared can be cyclized under mild acidic conditions into 1,5,6-trisubstituted indole derivatives (K. Kranjc, M. Kočevar, *Tetrahedron* 2008, *64*, 45).

The Diels−Alder reaction of *2H*-pyran-2-ones with a series of *N*-substituted maleimides yielding derivatives of fused bicyclo[2.2.2]octene, can be carried out in aqueous solutions and under microwave irradiation conditions. If sensitive functional groups are present as part of the starting compounds, it is more convenient to perform the reaction in the absence of any solvent (K. Kranjc, M. Kočevar, *Heterocycles* 2007, *73*, 481). A related type of products was prepared starting from variously substituted bicyclo[2.2.2]oct-7-ene-2*exo*,3*exo*,5*exo*,6*exo*-tetracarboxylic acid 2,3;5,6-dianhydrides and a set of hydrazines. In an aqueous solution under microwave irradiation conditions the corresponding fused *N*-aminosuccinimides were formed with high yields. The starting derivative, possessing an additional acetyl moiety, also reacted at this additional group to give the corresponding hydrazono derivatives of *N*-aminosuccinimides as the sole products (J. Hren, K. Kranjc, S. Polanc, M. Kočevar, *Heterocycles* 2007, *72*, 399).

2*H*-Pyran-2-ones were proven to be very useful synthons for the transformations into a variety of heterocyclic systems as well. In particular, we have investigated their conversion into derivatives of pyridazine, which were further used as substrates for the preparation of a series of heterocyclic compounds, especially when using ammonium cerium(IV) nitrate (CAN) as an oxidant. Here we succeeded to isolate an intermediate, thus enabling the possibility of clarification for the whole transformation (F. Požgan, S. Polanc, M. Kočevar, *Tetrahedron* 2006, *62*, 9718; F. Požgan, S. Kafka, S. Polanc, M. Kočevar, *Heterocycles* 2006, *70*, 235). We have also investigated the migration of a 2*H*-pyran-2-one unit under the condition of the Schmidt reaction and were the first to detect a migration of such a group in the above reaction (F. Požgan, M. Krejan, S. Polanc, M. Kočevar, *Heterocycles* 2006, *69*, 123).

Finally, we synthesized a series of 3-benzoylamino derivatives of 5- to 8-membered cycloalka[*b*]pyran-2-ones and 2*H*-pyran-2-ones by applying our previously described methods starting from the appropriate alkanones, *N*,*N*-dimethylformamide dimethyl acetal (DMFDMA) and hippuric acid in the presence of a large excess of acetic anhydride (F. Požgan, K. Kranjc, V. Kepe, S. Polanc, M. Kočevar, *ARKIVOC* 2007, (*viii*), 97).

We also investigated the reactivity of some simple alpha-amino acid derivatives (derivatives of oxazol-5(4*H*)-one, 2-aminopropenoic acid and diaminomaleonitrile) and their applicability in the synthesis of some natural product analogues and some other heterocyclic compounds. Two simple approaches to substituted 2-amino-3-(vinylamino)propenoates were elaborated from diaminomaleonitrile, 4-ethoxymethylene-2-phenyl-5(4*H*)-oxazolone, and alkyl or cycloalkyl alcoholes (T. Trček, B. Verček, *Acta Chim. Slov*. 2005, *52*, 171). We developed a new method for the synthesis of a series of alkyl 3-(imidazol-1-yl)propenoates starting from *N*-oxazolidenmethyl substituted diaminomaleonitrile (T. Trček, B. Verček, *ARKIVOC* 2005, (*xiv*), 96). We also investigated four ‘one-pot’ procedures for the preparation of highly functionalized imidazo[1,5-*a*]pyrazines based on the conversions of two diaminomaleonitrile and two imidazole derivatives (T. Trček, B. Verček, *Synthesis* 2006, 3437). Some benzoylaminomethyl substituted triazoloazines were prepared by reactions between acylglycines and heteroarylhydrazines (I. Mušič, B. Verček, *Heterocycl. Commun*. 2005, *11*, 321). 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 *via* ethyl 2-(benzoylamino)-3-(phenylhydrazono)propanoates has been described (K. Čuček, A. Golobič, B. Verček, *Heterocycles* 2007, *73*, 555). In addition, a number of ethyl 3-(benzoylamino)-1*H*-indole-2-carboxylates were prepared by heating ethyl 2-(benzoylamino)-3-(phenylhydrazono)propanoates with polyphosphoric acid (K. Čuček, B. Verček, *Synthesis* 2008, 1741).

We were also involved in the EU program COST D24/007/02 programme which consisted of eight research teams aiming at the development of novel catalytic and selective methods (especially hydrogenations and oxidations) under heterogeneous catalytic conditions. Our role within this research team was to develop industrially relevant substrates (α,β-didehydro-α-amino acid derivatives and unsaturated carbonyl compounds) that could not be transformed further by conventional methods, and would be used to fine-tune newly developed techniques for enantioselective reductions and oxidations. Within this framework we have investigated preparation of platinum colloids modified by chiral ligand synphos with the goal to obtain catalytic nanomaterial. The colloids were subsequently embedded in silica to form a heterogeneous catalyst. These colloids, both as 'quasi-homogeneous catalysts' (or soluble heterogeneous catalysts) and embedded in silica (heterogeneous catalysts) were employed in the selective hydrogenolysis of highly sterically constrained bicyclo[2.2.2]oct-7-enes and hydrogenation of ethyl pyruvate. We would like to stress that our methodology opens up new aspects of chemistry of bicyclo[2.2.2]octenes, where instead of the expected hydrogenation of the double bond its breaking occurs, thus producing highly substituted multifunctional cyclohexane building blocks (F. Neațu, A. Kraynov, V. I. Pârvulescu, K. Kranjc, M. Kočevar, V. Ratovelomanana-Vidal, R. Richards, *Nanotechnology* 2008, *19*, art. no. 225702 (8 pp)). The second catalyst for the selective hydrogenolysis of the above substrates was prepared from Fe_3O_4 colloids, modified with the chiral ligand cinchonidine and finally embedded in silica (F. Neațu, A. Kraynov, L. D'Souza, V. I. Pârvulescu, K. Kranjc, M. Kočevar, V. Kuncser, R. Richards, *Appl. catal., A Gen.* 2008, *346*, 28).

We have also published a review about the synthesis and transformations of fused bicyclo[2.2.2]octenes (J. Hren, S. Polanc, M. Kočevar, *ARKIVOC* 2008, (*i*), 209).

Organic BF_2 chelates appeared to be interesting intermediates in organic transformations. We prepared and studied various transformations of some BF_2 chelates. We have explored the previously unknown direct conversion of 5,6-disubstituted 2,2-difluoro-4-alkoxy-1,3,2-dioxaborinanes to 2,2-difluoro-4-alkylamino analogues with a variety of amines. Also, we have demonstrated a useful method for the synthesis of β-keto amides and β-enamino carboxamides in two overall steps with good yields starting from easily accessible starting materials. This chemo- and regioselective approach could be the method of choice for the preparation of such systems (B. Štefane, S. Polanc, *Synlett* 2004, 698; *Tetrahedron* 2007, *63*, 10902).

Oxidations of aryl and heteroarylhydrazines and hydrazides with CAN lead to the formation of various products. The reaction pathway strongly depends on the nature of the substrate. In most cases, hydrocarbons or alkoxy derivatives were isolated as the final products. When deuterated solvents such as methanol-d_4 or acetonitrile-d_3 were used, a regiospecific incorporation of deuterium was achieved (B. Štefane, S. Polanc, *Synlett* 2008, 1279).

Studies concerning the diazene chemistry showed that dialkyl diazenedicarboxylate reacted with 4-fluorophenol in the presence of $ZrCl_4$ to give the derivatives of 2-chlorophenol, aminated at the position 4 with regard to the OH group (S. Bombek, F. Požgan, M. Kočevar, S. Polanc, *J. Org. Chem.* 2004, *69*, 2224). Furthermore, reactions of methyl cyclohexylaminocarbonyldiazenedicarboxylate and methyl (2-chloroethylamino)carbonyldiazenedicarboxylate with 1,3-diketones, β-keto esters and β-keto amides in the presence of sodium acetate led to the corresponding Michael adducts as stable products. The latter were treated with ion-exchange resin (Dowex) to give substituted 2-imidazolin-2-ones. The influence of the base is crucial for the outcome of the reaction. In the presence of DBN, Michael adducts further reacted. Namely, they cyclized into 2-imidazolidinones and were then quantitatively transformed with Dowex to 2-imidazolin-2-ones as the final products. *N*-Phenylacetoacetamide reacted with the above

mentioned diazenes in the presence of DBN to give the mixture of two products. They were separately treated with CF_3CO_2D followed by elimination of water using NMR. The application of β-keto amides, particularly acetoacetamide and *N*-phenylacetoacetamide, for the formation of imidazolones is important in the light of an ever growing interest in biologically active amides of imidazolecarboxylic acids (S. Bombek, F. Požgan, M. Kočevar, S. Polanc, *New J. Chem.* 2005, *29*, 948). Very recently we have described the first example of the use of a $ZrBr_4$/diazene mixture for the selective bromination of various phenols, aromatic ethers and anilines. The method is completely regioselective thus offering numerous synthetic applications. The reaction takes place under mild reaction conditions and the bromine atom enters first at the *para* unsubstituted position with respect to the OH, OR or NR_2 group of the corresponding activated aromatic substrate. Less-reactive compounds such as toluene, phenyl acetate, benzonitrile, and trifluoromethylbenzene, remain intact under the same conditions. Mild reaction conditions, a relatively rapid conversion, good-to-excellent yields, and the selectivity profile are notable characteristics of this protocol (T. Stropnik, S. Bombek, M. Kočevar, S. Polanc, *Tetrahedron Lett.* 2008, *49*, 1729).

We have also evaluated the potential of using tetramethylammonium chloride as an alternative methylating agent for phenols under microwave-assisted conditions. We found that many simple phenols can be methylated in the presence of K_2CO_3, whereas some other less-reactive phenols require the presence of the more reactive Cs_2CO_3 (N. Maraš, S. Polanc, M. Kočevar, *Tetrahedron* 2008, *64*, 11618).

The studies concerning 1,3-diaryltriazenes revealed that triethylammonium triazenides smoothly reacted at room temperature with alkyl propiolates to give the alkoxycarbonylvinyltriethylammonium triazenides in high yields. The same compounds were isolated if triethylamine was added to a mixture of alkyl propiolate and a selected triazene in acetonitrile. The alkoxycarbonylvinyltriethylammonium triazenides are prone to trans-esterification. The triazenide counterion plays an important role in this process (A. Virag, A. Meden, M. Kočevar, S. Polanc, *J. Org. Chem.* 2006, *71*, 4014).

In collaboration with the research group of Dr. M. Osmak (Institute Ruđer Bošković, Zagreb) cytotoxicity of several compounds was studied. Very good results were obtained with *N*-(2-chloroethyl)-2-(2,3,4,5,6-pentafluorophenyl)diazenecarboxamide. IC_{50} for this compound is within the range of 16−42 μM in several carcinoma cells. It should be mentioned that this compound does not only inhibit the growth of parental cells but also the growth of drug-resistant cell lines, resistant to cisplatin, vincristine and doxorubicin (T. Čimbora-Zovko, S. Bombek, J. Košmrlj, L. Kovačič, S. Polanc, A. Katalinić, M. Osmak, *Drug Develop. Res.* 2004, *61*, 95). The fact that diazenes selectively oxidize thiols to disulfides is also reflected in their influence on intracellular glutathione level. Furthermore, several diazenes exhibit strong cytotoxicity against various human parental tumour cells and their drug-resistant sublines (S. Polanc, *J. Heterocycl. Chem.* 2005, *42*, 401). Examination of biological activity of diazenes also revealed that structurally similar compounds show significantly different cytotoxicity which seems to be related to the difference in the basicity of certain fragments in the molecule (S. Jakopec, K. Dubravčić, A. Brozović, S. Polanc, M. Osmak, *Cell Biology and Toxicology* 2006, *22*, 61). In addition, *N*-phenyl-2-(2-pyridinyl)diazenecarboxamide caused a type of programmed cell death of human cervical carcinoma cells which can be considered as 'apoptosis-like' (S. Jakopec, K. Dubravčić, S. Polanc, J. Košmrlj, M. Osmak, *Toxicology in Vitro* 2006, *20*, 217). A series of 16 diazenes were also screened towards four human leukemic cell lines (NALM-1, JURKAT, HL-60 and K-562). Eleven of them were cytotoxic towards leukemic cells, but did not affect normal resting human peripheral blood mononuclear cells. Eight diazenes affected neither normal dividing cells (nor Con-A-stimulated PBMC and 3T3 fibroblasts). Thus, the

observed selective cytotoxicity of these diazenes is a promising new potential for the treatment of leukemia patients (I. Martin-Kleiner, S. Bombek, J. Košmrlj, B. Čupić, T. Čimbora-Zovko, S. Jakopec, S. Polanc, M. Osmak, J. Gabrilovac, *Toxicology in Vitro* 2007, *21*, 1453).

D-Alanine-D-alanine ligase (Ddl) catalyzes the biosynthesis of an essential bacterial peptidoglycan precursor D-alanyl-D-alanine and represents an important target for the development of new antibacterial drugs. Following this goal, we prepared a series of diazenedicarboxamides and studied their activity as inhibitors of DdlB from *E. coli*. Thirteen compounds were found to be better inhibitors than D-cycloserine, and five of them had IC_{50} values below 50 μM. These inhibitors are structurally distinct from both ADP and D-alanine, so we expect that they inhibit Ddl by a novel binding mode. As many diazenedicarboxamides also have *in vitro* antimicrobial activities, they constitute a promising starting point for further investigations. The above studies were accomplished in collaboration with Prof. S. Gobec, Faculty of Pharmacy, University of Ljubljana and Prof. I. Chopra, University of Leeds (A. Kovač, V. Majce, R. Lenaršič, S. Bombek, J. M. Bostock, I. Chopra, S. Polanc, S. Gobec, *Bioorg. Med. Chem. Lett.* 2007, *17*, 2047; Patent application: S. Gobec, A. Kovač, A. Brajić, S. Pečar, J. Bostock, I. Chopra, R. Lenaršič, S. Bombek, M. Kočevar, S. Polanc*, Diazenedicarboxamides as inhibitors of D-alanine: D-alanine ligaes (Ddl) : European patent no. EP07468010, publication date: 07. Avgust 2007*. Munich: European Patent Organisation, 2007.).

The connection of two active molecules across an easily released bridge as a new type of potentially active molecules has been studied in collaboration with Prof. J. Vinšová, Faculty of Pharmacy, Charles University, Hradec Králové. The synthesis was based on derivatives that originated from isonicotinoyl hydrazide (INH), pyrazinamide (PZA), *para*-aminosalicylic acid, ethambutol, and ciprofloxacin. The lipophilicity, hydrolytic stability of the compounds and antituberculotic activity, as well as the structure-lipophilicity and structure-activity relationships were studied. It was found out that the rate of hydrolysis of the new products depends on the fragments involved in the molecule. The anti-tuberculosis activity was evaluated against *M. tuberculosis H37Rv* and three non-tuberculous strains. Three new compounds demonstrate higher activity against non-tuberculous strains than INH or PZA which were used as internal standards. In addition, the hydrolysis of new compounds ensures a prolonged liberation of active components (A. Imramovský, S. Polanc, J. Vinšová, M. Kočevar, J. Jampílek, Z. Rečková, J. Kaustová, *Bioorg. Med. Chem.* 2007, *15*, 2551).

In collaboration with the research group of Prof. Dr. S. Kafka and Prof. Dr. A. Klásek (Tomas Bata University in Zlin, Czech Republic; bilateral projects: BI-CZ/03-04-5, BI-CZ/05-06/009, BI-CZ/07-08-018) we continued our research on quinoline-2,4(1*H*,2*H*)-diones in the field of corresponding 3-hydroxy, 3-thio, and 3-amino analogues as follows: We have found out that some 3-hydroxy-2,4(1*H*,3*H*)-diones in alkaline aqueous media rearrange into structurally diverse products. Thus, 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 was accompanied by the formation of two by-products of spiro[2*H*-indol]-3(1*H*)-one skeletons. The structures of these were elucidated by NMR, MS, and confirmed by X-ray diffraction. Structural analysis of spiro[2*H*-indol]-3(1*H*)-ones is important as this structural motif has been found in some natural products, and is a key part of some biologically active molecules and compounds having photochromic properties (J. Košmrlj, S. Kafka, I. Leban, M. Grad, *Magn. Reson. Chem.* 2007, *45*, 700).

We also studied the reactivity of derivatives in which the 3-hydroxy group is protected as an ester group. To this end, 3-hydroxyquinoline-2,4(1*H*,3*H*)-diones were transformed into furo[2,3-*c*]quinoline-2,4(3a*H*,5*H*)-diones by Wittig olefination with ethyl (triphenylphospho ranylidene)acetate ($Ph_3P{=}CHCO_2Et$), which in thermally-assisted base-catalyzed reaction re-

arranged into furo[3,4-*c*]quinoline-3,4(1*H*,5*H*)-diones. The mechanism of the rearrangement has been proposed and the results were disclosed in a preliminary communication (S. Kafka, J. Košmrlj, A. Klásek, A. Pevec, *Tetrahedron Lett.* 2008, *49*, 90).

In connection to 3-thio analogues, we have studied novel tandem hydration of α-thiocyanatoketones to thiocarbamates followed by in situ cyclodehydration to fused 2-oxo-3-thiazolines. The reaction has been applied to the synthesis of [1,3]thiazolo[5,4-*c*]quinoline-2,4(3a*H*,5*H*)-diones from 3-thiocyanatoquinoline-2,4(3a*H*,5*H*)-diones. A limited number of strategies for the preparation of fused 2-oxo-3-thiazolines are precedent in the literature, and our contribution represents a new method. It is worth to note that the above mentioned structures are important: for example, related 2-arylthiazolo[4,5-*c*]quinolin-4(5*H*)-ones have recently been found to posses high affinity for the GABA receptor (A. Klásek, V. Mrkvička, A. Pevec, J. Košmrlj, *J. Org. Chem.* 2004, *69*, 5646).

Regarding 3-aminoanalogues, selected 3-aminoquinoline-2,4(1*H*,3*H*)-diones were transformed into pyrrolo[2,3-*c*]quinoline-2,4(3a*H*,5*H*)-diones. For this, two alternative approaches were studied: inter- and intramolecular Wittig olefination. In preliminary experiments we confirmed that pyrrolo[2,3-*c*]quinoline-2,4(3a*H*,5*H*)-diones in a base-catalyzed reaction isomerize into corresponding pyrrolo[3,4-*c*]quinoline-3,4(2*H*,5*H*)-diones. None of these skeletons have previously been described in literature (S. Kafka, A. Klásek, J. Polis, V. Rosenbreierová, C. Palík, V. Mrkvička, J. Košmrlj, *Tetrahedron* 2008, *64*, 4387).

We found out that *S*-(3-alkyl/aryl-2,4-dioxo-1,2,3,4-tetrahydroquinolin-3-yl)thiocarbamates thermally reacted to form 4-hydroxy-1*H*-quinolin-2-ones. Under the same reaction conditions, 3a-alkyl/aryl-[1,3]thiazolo[5,4-*c*]quinoline-2,4(3a*H*,5*H*)-diones reacted to yield one of two different types of products, depending on the nature of the substituent at the 5th position. These, substituted with an alkyl or aryl group produced 4-amino-3-alkyl/aryl-1*H*-quinolin-2-ones, whereas the N-5 unsubstituted analogues rearranged to form novel 6*H*-thiazolo[3,4-*c*]quinazoline-3,5-diones in high yields. The reaction mechanisms for the above transformations are discussed (V. Mrkvička, A. Klásek, R. Kimmel, A. Pevec, J. Košmrlj, *ARKIVOC* 2008, (*xiv*), 289).

We were successful in acquiring preliminary results in connection with the research proposal for the program P1-0230 Organic chemistry: Synthesis, Structure and Application (2009-13), as follows. Azoamides, previously established as bioactive intracellular GSH-depleting agents, were decorated with a terminal alkyne moiety to propargyl-functionalized azoamides and then by copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) transformed into different ligand-arm functionalized azoamides. Azides, having ligand-arms amenable for binding to platinum(II), were selected for this study. As for fragile azoamides propargyl-functionalized azoamides the typically employed reaction conditions for CuAAC failed, several alternative solvents and copper catalysts were tested. Excellent results were obtained with copper(II) sulfate pentahydrate/metallic copper and especially with heterogeneous catalysts such as copper-in-charcoal, cupric oxide, and cuprous oxide. By employing heterogeneous catalysts, the desired products were obtained in almost quantitative yields by a simple three-step ‘stir–filter–evaporate’ protocol with no, or negligible contamination with copper impurities. This is of particular importance as ligand-arm functionalized azoamides have been designed for coordination. This research outlines a modular entry enabling the preparation of diverse ligand arm-functionalized azoamides. Employing suitable ligand arms, azoamides will be explored as potential bioactive ligands in novel cisplatin analogues, hybrid molecules with a potential dual mode of action in anticancer treatment. Moreover, the results presented in this work will find broader application, especially in automated combinatorial “click” chemistry (D. Urankar, J. Košmrlj, *J. Comb. Chem.* 2008, *10*, 981).

The ethylidenemalononitrile side-chain in {1-[6-(dimethylamino)-2-naphthyl]ethylidene}-malononitrile (DDNP) was elaborated into a substituted pyridine ring in a two-step process. Chloroimidate intermediate in the reaction of a nitrile group with HCl in alcoholic solution was trapped in the form of 2-chloro-4-[6-(dimethylamino)-2-naphthyl]nicotinonitrile, thus proving its existence in the Pinner synthesis. It also served as the starting material for the preparation of several derivatives obtained through nucleophilic displacement of chlorine. The structure of 2-methylamino derivative was also proven by X-ray analysis (P. Škofic, C. Dambrot, M. Koželj, A. Golobič, J. R. Barrio, A. Petrič, *Acta Chim. Slov.* 2005, *52*, 391)

In collaboration with colleagues from the Faculty of Medicine UL we have demonstrated that FDDNP labeling reliably predicts birefringence in Congo red stained histological sections in particular microscopic structures in classical amyloid forming disorders like Alzheimer's disease, cerebral amyloid angiopathy and transmissible spongiform encelopathies (A. Šmid, T. D. Vovko, M. Popović, A. Petrič, V. Kepe, J. R. Barrio, G. Vidmar, M. Bresjanac, *Brain Pathol.* 2006, *16*, 124). 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 (J. Liu, V. Kepe, A. Žabjek, A. Petrič, H. C. Padgett, N. Satyamurthy, J. R. Barrio, *Mol. Imaging Biol.* 2007, *9*, 6).

Our research has brought forward new knowledge on the synthesis of complex compounds, especially on the synthesis of novel types of building-blocks and on the development of new synthetic methods, including heterogeneous chemoselective syntheses. Novel reactions in organic synthesis have been thoroughly investigated and explained; on the other hand, we have also synthesized some new biologically active compounds.

OTHER RELEVANT ACHIEVEMENTS

The aim of the research project *From multifunctional building blocks to biologically-active compounds (J1-6693-0103)* was to develop synthetic approaches and further design of differently substituted multifunctional building blocks that could be subsequently used as model compounds for developing novel methods in the field of organic chemistry (selective syntheses), as well as the preparation of potentially biologically-active intermediates, that could be introduced into more complex compounds. This research programme was a part of our research activity within the international program EU COST D24 Action Sustainable Chemical Processes: Stereoselective Transition Metal-Catalysed Reactions (D24/0007/02: Synthesis and Application of New Ligands for Asymmetric Heterogeneous Catalysis).

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4. F. Požgan, J. Roger, H. Doucet, *ChemSusChem.* 2008, *1*, 404.

PLENARY AND INVITED LECTURES

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

OTHER ACTIVITIES

M. Kočevar is a National Representative of IUPAC Organic and Biomolecular Chemistry Division (III) Committee (for the period 2008−2009) and member of the Management Committee COST D40 Innovative Catalysis: New Processes and Selectivities (2006−2011). *Editorial activity:* J. Košmrlj was editor-in-chief (2003−2005) of the *Acta Chimica Slovenica* (ACS), K. Kranjc is member of the editorial board (2007−) of ACS, M. Kočevar is a member of editorial board of *Periodica polytechnica. Chemical engineering* (2003−); he was also a member of editorial board of *Slovenski veliki leksikon (Slovene Comprehensive Lexicon)*. S. Polanc is a member of editorial board of the *Topics in heterocyclic chemistry* (2008−).

AWARDS

A. Petrič and J. Košmrlj were awarded (together with A. Pavko) the Maks Samec award for popularization of studies at the Faculty of Chemistry and Chemical Technology, University of Ljubljana.

KEMIJSKO INŽENIRSTVO
CHEMICAL ENGINEERING

PROGRAMSKA SKUPINA / RESEARCH PROGRAMME GROUP

P2–0191

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Dušan Komel
Janez Malovrh

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

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.*

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.

Z obsežnim eksperimentalnim delom na koloni s perforirano ploščo smo ustvarili podatkovno bazo deleža plina v raztopinah karboksimetil celuloze (CMC) in ksantana. Podatkovno bazo smo analizirali z v literaturi uveljavljenima modeloma (angl.: drift-flux model in angl.: slip velocity model) in konfrontirali 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.

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

Na področju mikroreaktorske tehnologije smo študirali razgradnjo 4-klorofenola v mikroreaktorju z dvokovinskim Pd/Fe katalizatorjem, ki daje možnost in situ odstranjevanja nevarnih

snovi. Ugotovili smo, da je proces v pretočnem mikroreaktorskem sistemu pri sobni temperaturi le delno učinkovit, a smo s povišanjem temperature na 60 °C povečali konverzijo 4-klorofenola pri danem enkratnem pretoku skozi reaktor na 90 %. Razvili smo dvodimenzionalni matematični model, ki vključuje konvekcijo, difuzijo in katalitsko reakcijo psevdo-prvega reda, s katerim smo analizirali eksperimentalne podatke in napovedali obnašanje reaktorja.

Predmet poglobljene raziskave je bila stabilizacija disperzij, pridobljenih na osnovi oborjenih kalcijevih karbonatov s komercialnimi natrijevimi poliakrilatnimi disperzanti. Rezultati so pokazali, da sestava matične lužnice, posebno aktivnost Ca^{2+} ionov, močno vpliva na vse procese, ki so pomembni za stabilizacijo disperzije; od začetnega naboja površine $CaCO_3$ v osnovnih disperzijah do regulacije naboja in stabilizacije disperzije. Rastoča vloga protiionske kondenzacije dosežena v Ca^{2+} bogatih raztopinah omejuje pogoje primerne za regulacijo površinskega naboja preko adsorpcije disperzanta na optimalno pH območje med 8 in 11. Analiza stabilnosti disperzije, podprta s klasično DLVO teorijo koloidne stabilnosti in podprta z eksperimentalnimi rezultati (porazdelitev velikosti delcev), je pokazala, da so pogoji za optimalno stabilnost disperzije doseženi z majhnimi količinami disperzanta v območju pH vrednost med 9 in 11.

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.

Opredeljena je bila metoda za napoved padca tlaka, ki nastane pri pretoku PA6 skozi pleteni filter in šobo, ki sta sestavna dela šobnega paketa za predenje najlona. Identificirani in analizirani so bili dejavniki, ki jih je treba pri napovedi padca tlaka upoštevati. Delo obravnava določitev reoloških lastnosti PA6 in opis reološkega obnašanja PA6 s Crossovim viskoznim modelom in s K-BKZ viskoelastičnim integralnim modelom, matematične modele za napoved padca tlaka skozi šobe in pletene filtre ter primerjavo rezultatov z eksperimentalnimi podatki padca tlaka izmerjenimi na industrijski pilotni liniji.

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 nenewtonski 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. Kvantificiran je bil 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. Doseženi 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, preučiti možnost uporabe nenasičenega poliuretana v gumeni zmesi z naravnim kavčukom, butadienskim kavčukom in z mešanico naravnega in butadienskega kavčuka z namenom izboljšave lastnosti gumene zmesi, raziskati mešljivost polibutadienskega kavčuka (BR), polistiren-ko-butadienskega kavčuka in naravnega kavčuka (NR), razviti testno metodo za določevanje abrazijske odpornosti zobatega pogonskega jermena, preučiti in modelirati kinetiko sinteze fenol-formaldehidnih smol in melaminsko- formaldehidnih smol, preučiti in modelirati kinetiko zamreževanja melaminsko-formaldehidnih smol, osvojiti tehnologijo priprave melaminskih pen, preučiti in modelirati kinetiko radikalske polimerizacije dialil tereftalata, ki vključuje tudi difuzijo monomera v polimeru, preučiti sintezo vodnih poliuretanskih disperzij, preučiti vpliv sestave poliuretana na lastnosti poliuretanskih filmov, preučiti sintezo hibridnih akrilatno-poliuiretanskih vodnih disperzij s polšaržno emulzijsko polimerizacijo akrilatnih monomerov v različnih poliuretanskih disperzijah, načrtovati lastnosti akrilatno-poliuretanskih veziv in njihovih filmov, raziskati kinetiko emulzijske polimerizacije akrilatnih monomerov v prisotnosti poliuretanskih kali, raziskati suspenzijsko polimerizacijo akrilatov, 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.

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 sredotočili na selekcijo in optimizacijo gojišč za produkcijo biomase ter farmacevtrsko aktivnih snovi ter možnosti izkoriščanja industrijskih odpadkov. (2) kontrolirano gojenje v bioreaktorju za sterilizirana trdna gojišča (solid-state) iz agroživilske in lesne industrije ter (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 astoržev, 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

Bioremediacija: Raziskave so potekale z namenom pripraviti mešanico ligninoliticnih encimov za razbarvanje sintetičnih barvil, ki so običajno prisotna v odpadnih vodah iz tekstilne industrije. Razbarvanje sintetičnega organskega azo barvila RO16 smo proučevali z glivo bele trohnobe *Irpex lacteus* v različnih laboratorijskih bioreaktorjih, od katerih je bil najučinkovitejši kapalni reaktor. Ugotovili smo, da pri razbarvanju sodelujejo ekstracelularni ligninolitočni encimi, kakor tudi encimi vezani na micelij. Hitrost razbarvanja smo opisali s kinetično enačbo spremenljivega reda od 0,7 pri nižjih koncentracijah barvila do 1,0 pri višjih koncentracijah barvila.

Raziskave smo nadaljevali z glivo *Ceriporiopsis subvermispora,* ki je znana po sintezi lakaz in mangan peroksidaz za uporabo v industriji celuloze. Postopek za proizvodnjo encimov v stacionarnih kulturah je bil optimiran glede na vrsto sladkorja kot vira ogljika, vrsto lesa kot induktorja in nosilca za imobilizacijo kulture ter dodanega vira dušika. Na osnovi različnih pogojev gojenja so bili pripravljeni mediji s prebitkom lakaz, prebitkom mangan peroksidaz ter enakostjo obeh aktivnosti. Ti so bili v nadaljevanju raziskav uporabljeni za razbarvanje strukturno različnih organskih barvil kot so RBBR, CuP in RO16. Ugotovljeno je bilo da posamezni encimi bolje razbarvajo barvila specifičnih kemijskih struktur.

Vpliv vrste nosilca, sladkorja in dušika na sintezo lakaz in mangan peroksidaz smo proučevali z glivo *Dichomitus squalens*. Bukov les in slama sta bila najboljša induktorja, fruktoza najboljši vir ogljika, dodani dušik pa je ugodno vplival na razvoj aktivnosti. Nastale encimske mešanice smo testirali pri razbarvanju izbranih barvil in ugotovili, da je bil učinek razbarvanja po 10 urah 62 % za RBBR, 50 % za bakrov(II)ftalocianin (CuP) in 19 % za reaktivno oranžno 16 (RO16).

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:

- Raziskave na področju bioremediacije

ZNANSTVENI DOSEŽKI

Akrilatno poliuretanske hibridne emulzije za premaze: sinteza, karakterizacija in uporabnost: Raziskovalno delo je zajemalo temeljne in aplikativne raziskave, saj je bil končni cilj projekta razviti nov, okolju prijazni, hibridni premaz za kovino na vodni osnovi, ki bo izkazoval prednosti AC in PU komponente. Iz omenjenih raziskav tako izhaja več dosežkov (publicistika, aplikativni rezultati, učinki aplikativnih rezultatov). Raziskovali smo kinetiko nastanka vo-

dne AC-PU hibridne emulzije. Hibridne emulzije smo pripravili s polšaržno emulzijsko polimerizacijo metil metakrilata v prisotnosti predhodno sintetiziranih PU disperzij z različnimi sestavami in lastnostmi. Trdoto PU smo spreminjali s spreminjanjem kemijske strukture in molekulske mase poliola ter z dodatkom butandiola. Raziskovali smo vpliv različnih PU delcev na hitrost polimerizacije, na velikost hibridnih delcev in njihovo porazdelitev, na totalno število delcev v reaktorju in na povprečno število radikalov na delec. Med vodenjem emulzijske polimerizacije smo spreminjali hitrost dodajanja monomerne predemulzije v reaktor in študirali njen vpliv na proces. Ugotovili smo, da so PU delci, ki so bili pripravljeni iz tršega PU, hitreje nabrekali z AC komponento, predno so v sistemu nastopili pogoji pomanjkanja monomera. V pogojih pomanjkanja monomera so bile razlike med serijami z različnimi PU kalmi minimalne. Povprečna velikost delcev je med procesom naraščala, njihovo število pa je bilo konstantno in istega velikostnega reda kot število PU kali v začetni polnitvi. Povprečno število radikalov na hibriden delec je naraščalo, zato smo kinetiko procesa opisali s kinetičnim modelom, ki upošteva fiksno koncentracijo radikalov. Ker je bilo ugotovljeno, da dodatek butil akrilata v AC komponento omogoča pripravo veziv, ki dajejo boljše mehanske lastnosti premazu, smo v nadaljevanju preučevali še kinetiko polšaržne emulzijske kopolimerizacije metilmetakrilata in butilakrilata v prisotnosti PU disperzij. Preučevali smo tudi vpliv sestave AC in PU komponente na aplikativne lastnosti hibridnih emulzij, na morfologijo hibridnih delcev ter na mehanske lastnosti filmov. Ugotovili smo, katera sestava emulzije je najprimernejša za izdelavo premaza za kovino. Rezultati raziskav imajo velik pomen za slovensko industrijo premazov. Z znanstvenega stališča pa se vplivi kažejo v citiranosti objav (v zadnjih štirih letih 21 citatov). Rezultati raziskav so bili predstavljeni na mednarodnih konferencah, v okviru tehnološke mreže in platforme ter objavljeni v treh člankih: *ŠEBENIK, Urška, KRAJNC, Matjaž. Seeded semibatch emulsion copolymerization of methyl methacrylate and butyl acrylate using polyurethane dispersion : effect of soft segment length on kinetics. Colloids surf., A Physicochem. eng. asp., 2004, vol. 233, no. 1/3, str. 51–62., ŠEBENIK, Urška, KRAJNC, Matjaž. Semibatch emulsion polymerization of methyl methacrylate using different polyurethane particles. J. polym. sci., Part A, Polym. chem., 2005, vol. 43, no. 4, str. 844–858.* in *ŠEBENIK, Urška, KRAJNC, Matjaž. Properties of acrylic-polyurethane hybrid emulsions synthesized by the semibatch emulsion copolymerization of acrylates using different polyurethane particles. J. polym. sci., Part A, Polym. chem., 2005, vol. 43, no. 18, str. 4050–4069.*

Kinetika vulkanizacije in prenos toplote v 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. 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. Tudi 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. 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. Rezultati raziskave omogočajo fundamentalno razumevanje kompleksne reakcijske sheme in transporta toplote med vulkanizacijo elastomerov. Postavljeni model omogoča optimizacijo proizvodne linije za gumene izdelke. Vpliv rezultatov se kaže v implementaciji v proizvodnji, kjer smo uspeli skrajšati procesni čas za 40 %. Rezultati so bili predstavljeni na mednarodnih konferencah, v okviru tehnološke mreže in platforme ter objavljeni v treh člankih: *LIKOZAR, Blaž, KRAJNC, Matjaž. Temperature dependent dynamic mechanical properties of hydrogenated nitrile butadiene rubber and the effect of peroxide cross-linkers. E-polymers., 2007, no. 131, str. 1–20.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Kinetic and heat transfer modelling 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.* in *LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Modelling of dynamic mechanical properties of vulcanized fluoroelastomer. Polym. eng. sci., 2007, vol. 47, no. 12, str. 2085–2094.*

Razgradnja 4-klorofenola v pretočnem mikroreaktorju z dvokovinskim Pd/Fe katalizatorjem: Delo obravnava razgradnjo 4-klorofenola v pretočnem mikroreaktorju z dvokovinskim Pd/Fe katalizatorjem, ki daje možnost in situ odstranjevanja nevarnih snovi. Pri enkratem pretoku skozi reaktor smo uspeli doseči 90 % konverzijo 4-klorofenola. Razvili smo dvodimenzionalni matematični model, ki vključuje konvekcijo, difuzijo in katalitsko reakcijo psevdo-prvega reda, s katerim smo analizirali eksperimentalne podatke in napovedali obnašanje reaktorja. Model omogoča izračun kinetičnih konstant reakcije in natančno napoveduje eksperimentalno dobljene konverzije pri različnih pretokih reaktanta. Primerjava modela mikroreaktorja z idealnimi reaktorji pri uporabljenih obratovalnih pogojih izkazuje obnašanje idealnega cevnega reaktorja. Delo je bilo predstavljeno strokovni javnosti na konferenci in objavljeno v članku: *JOVANOVIĆ, Goran, ŽNIDARŠIČ PLAZL, Polona, SAKRITTICHAI, Ploenpun, AL-KHALDI, Khaled. Dechlorination of p-chlorophenol in microreactor with bimetallic Pd/Fe catalyst. Ind. Eng. Chem. Res., 2005, 44 (14), 5099–5106.*

Kontinuirna ekstrakcija reaktanta in produkta biotransformacije progesterona v etilacetat v sistemu mikrokanalov: V sistemu mikrokanalov smo uspešno izvedli kontinuirno ekstrakcijo reaktanta in produkta biotransformacije progesterona v etilacetat, kar predstavlja osnovo za postavitev integriranega bioprocesa. Na osnovi 3D modela, ki poleg konvekcije in difuzije vključuje hitrostni profil obeh kapljevin, smo pravilno napovedali izkoristke ekstrakcij pri različnih pretokih faz. Ključni pomen raziskovalnega dela je načrtovanje in uporaba kontinuirne ekstrakcije v sistemu mikrokanalov kot izjemno učinkovite alternative klasičnim zaključnim procesom v biotehnologiji in kemijski industriji, kar je pionirsko delo na tem področju. Delo je bilo objavljeno v ugledni mednarodni reviji Lab on a Chip, njegovi izsledki pa so bili vključeni v vabljeno predavanje na konferenci Symbiosis: science, industry & society v Barceloni l. 2007 I. Plazl: Studies at the microreactor scale. *ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Steroid extraction in a microchannel system: mathematical modelling and experiments. Lab chip, 2007, 7 (7), 883–889.*

Suspenzijska polimerizacija za sintezo mikrosfernih na pritisk občutljivih 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 (Tg) ter na reološke lastnosti polimera. Pri sintezah akrilatnih polimerov pogosto nastaja zaradi intramolekularnega in intermolekularnega prenosa aktivnega mesta na verigo polimera do nastanka razvejanih polimerov z dolgimi stranskimi verigami,

ki 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. Rezultati raziskav so služili razvoju industrijske proizvodnje PSA lepil in bili objavljeni v člankih: *KAJTNA, Jernej, KRAJNC, Matjaž, GOLOB, Janvit. The role of components in waterbased microsphere acrylic PSA adhesive properties. Macromol. symp., 2006, vol. 243, no. 1, str. 132–146.*, *KAJTNA, Jernej, LIKOZAR, Blaž, GOLOB, Janvit, KRAJNC, Matjaž. The influence of the polymerization on properties of an ethylacrylate/2-ethyl hexylacrylate pressure-sensitive adhesive suspension. Int. j. adhes. adhes., 2008, vol. 28, no. 7, str. 382–390.* in *KAJTNA, Jernej, ŠEBENIK, Urška, KRAJNC, Matjaž, GOLOB, Janvit. IR drying of water-based acrylic PSA adhesives. Dry. technol., 2008, vol. 26, no. 3, str. 323–333.*

DRUGI RELEVANTNI DOSEŽKI

Razvoj poliuretanskih vodnih disperzij, razvoj akrilatno-poliuretanskih hibridnih emulzij ter razvoj in tehnologija priprave poliuretansko-akrilatnega pokrivnega premaza na vodni osnovi za zaščito kovin: Razviti so bili sledeči novi izdelki in tehnologije za njihovo pripravo: (i) poliuretanska vodna disperzija, (ii) – akrilatno-poliuretanska hibridna vodna emulzija, (iii) pokrivni premaz na vodni osnovi za zaščito kovin pri ekstremnih pogojih. Na tematiki sta magistrirala magistrant in magistrantka, zaposlena v družbi Helios d.d..

Aplikativni rezultati: razvoj novega izdelka, razvoj novega tehnološkega procesa oz. tehnologije, pridobitev novih praktičnih znanj, informacij in veščin, pridobitev novih znanstvenih spoznanj

Učinki aplikativnih rezultatov: razvoj dodiplomskega izobraževanja, razvoj podiplomskega izobraževanja, razširitev ponudbe novih izdelkov/storitev na trgu, večja konkurenčna sposobnost, dvig izobrazbene strukture zaposlenih in varovanje okolja in trajnostni razvoj

Dosežek je bil predstavljen na številnih znanstvenih konferencah in v magistrskih delih: *ŠEBENIK, Urška, KRAJNC, Matjaž. Semibatch emulsion polymerization of methyl methacrylate using different polyurethane seed particles, 7th world congress of chemical engineering, Incorporating the 5th European congress of chemical engineering, SECC, Glasgow, Scotland, 10–14 July 2005.*, *ŠEBENIK, Urška, KRAJNC, Matjaž. Rheological properties of acrylic-polyurethane hybrid emulsions synthesized by semibatch emulsion polymerization of acrylates using different polyurethane seed particles, 2nd Annual European Rheology Conference, April 21–23, 2005, Grenoble, France.*, *ŠEBENIK, Urška, KRAJNC, Matjaž. Kinetics of methyl methacrylate polymerization in polyurethane dispersions, 9th Austrian Polymer Meeting, March 26–28 2008, Graz, Austria.*, *GLAVAČ, Alenka. Sinteza in karakterizacija poliuretanskih vodnih disperzij : magistrsko delo. Ljubljana, 2004.* ter *VEZOČNIK, Borut. Razvoj in tehnologija priprave poliuretansko-akrilatnega pokrivnega premaza na vodni osnovi za zaščito kovin : magistrsko delo. Ljubljana, 2006.*

Izboljšanje obstoječih izdelkov in proizvodnih procesov v gumarski industriji: V sodelovanju z gospodarsko družbo Goodyear E.P.E. smo: (i) skrajšali čas vulkanizacije gumenih izdelkov, (ii) optimizirali sestavo gumene zmesi, (iii) razvili testno aparaturo in metodo za testiranje abrazijske odpornosti pogonskega jermena, (iv) izboljšali mehanske lastnosti in abrazijsko odpornost pogonskega jermena.

Aplikativni rezultati: izboljšanje obstoječega izdelka, zboljšanje obstoječih proizvodnih metod in instrumentov oz. proizvodnih procesov

Učinki aplikativnih rezultatov: razvoj dodiplomskega izobraževanja, razvoj podiplomskega izobraževanja, razširitev ponudbe novih izdelkov/storitev na trgu, večja konkurenčna sposobnost, tehnološka razširitev/posodobitev dejavnosti in uvajanje novih tehnologij.

Dosežek je dokumentiran v številnih faznih poročilih za Goodyear E.P.E, ki so zavedena v COBISSu. ter predstavljen na več mednarodnih konferencah: *LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Hydrogenated acrylonitrile butadiene elastomer/coagent nanocomposites : [oral contribution], European polymer congress [also] epf, 2–6 july, 2007, Congress centre Bernardin, Portorož, Slovenia.*, *ŠEBENIK, Urška, ZUPANČIČ-VALANT, Andreja, MESEC, Aleš, KRAJNC, Matjaž. Investigation of rubber-rubber blends miscibility by RPA and modulated-temperature DSC, 2nd Annual European Rheology Conference, April 21–23, 2005, Grenoble, France.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Sulfur vulcanization of various BR/NR blends with TBBS and TBSI accelerators : heat transfer, kinetics and rheology, Polymer Reaction Engineering VI, May 21–26, 2006, Halifax, Nova Scotia, Canada.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Kinetic modelling of peroxide vulcanization of hydrogenated nitrile butadiene rubber, Hangzhou International Polymer Forum, Hangzhou, China, May 13–17, 2007.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Viscoelastic behavior of hydrogenated nitrile butadiene rubber and the effect of coagents, Hangzhou International Polymer Forum, Hangzhou, China, May 13–17, 2007.*, *LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Dynamic mechanical properties of hydrogenated nitrile butadiene rubber at various temperatures and their modelling, European polymer congress [also] epf, 2–6 july, 2007, Congress centre Bernardin, Portorož, Slovenia.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Determination of thermophysical properties of various elastomers, 9th Austrian Polymer Meeting, March 26–28, 2008, Graz, Austria.*

Razvoj PSA lepil: Razvita so bila nova in optimizirana obstoječa PSA lepila. Na tematiki je doktoriral doktorand, zaposlen v družbi Aero, d.d.

Aplikativni rezultati: razvoj novega izdelka, razvoj novega tehnološkega procesa oz. tehnologije, pridobitev novih praktičnih znanj, informacij in veščin, pridobitev novih znanstvenih spoznanj

Učinki aplikativnih rezultatov: razvoj dodiplomskega izobraževanja, razvoj podiplomskega izobraževanja, razširitev ponudbe novih izdelkov/storitev na trgu, večja konkurenčna sposobnost, dvig izobrazbene strukture zaposlenih in varovanje okolja in trajnostni razvoj

Dosežek je bil predstavljen na številnih znanstvenih konferencah: *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, 2007, str. [1–2].*, *KAJTNA, Jernej, GOLOB, Janvit, KRAJNC, Matjaž. The role of components in waterbased microsphere acrylic PSA adhesive properties. V: Polymer Reaction Engineering VI, May 21–26, 2006, Halifax, Nova Scotia, Canada. Program : ECI : Engineering Conferences International., 2006.*, *KAJTNA, Jernej, KRAJNC, Matjaž, GOLOB,*

Janvit. The effect of gel phase on adhesion properties of microsphere suspension based acrylic pressure sensitive adhesives. V: Hangzhou International Polymer Forum, Hangzhou, China, May 13–17, 2007. Advanced materials and reaction engineering., 2007., *KAJTNA, Jernej, ŠEBENIK, Urška, KRAJNC, Matjaž. Microsphere pressure sensitive adhesives : acrylic polymer/montmorillonite clay nanocomposite materials. V: 9th Austrian Polymer Meeting, March 26–28 2008, Graz, Austria, 2008.* in v doktorskem delu: *KAJTNA, Jernej. Suspenzijska polimerizacija in sušenje mikrosfernega akrilatnega lepila: doktorsko delo. Ljubljana, 2008.*

Koncentriranje aktivne farmacevtske učinkovine Lizinopril z reverzno ozmozo: Aktivno farmacevtsko učinkovino Lizinopril je po čiščenju z nizkotlačno tekočinsko kromatografijo potrebno koncentrirati. Reverzna ozmoza (RO) v zadnjem času uspešno nadomešča uparjanje. Uporabnost RO za koncentriranje smo pri različnih obratovalnih pogojih najprej preverili s poskusi v pilotnem merilu. Rezultati pilotnih poskusov so bili osnova za izračun potrebne površine membran ter za oceno investicijskih in obratovalnih stroškov industrijske naprave za RO in uparjalnika. Na osnovi teh rezultatov je bila načrtovana in postavljena industrijska naprava za RO. Dejanski investicijski in obratovalni stroški ter tekoče obratovanje so pokazali, da je bil prenos postopka v industrijsko merilo uspešen ter uporaba RO ekonomsko ugodnejša in zato upravičena.

Aplikativni rezultati: prenos obstoječih tehnologij v prakso in izboljšanje obstoječega proizvodnega procesa.

Učinki aplikativnih rezultatov: razvoj dodiplomskega izobraževanja, razvoj podiplomskega izobraževanja, tehnološka razširitev/posodobitev dejavnosti in uvajanje novih tehnologij.

Dosežek je dokumentiran v prispevku: *D. Senica, J. Ržen, M. Uštar, P. Drnovšek, S. Kogej, A. Pavko: Reverse osmosis to concentrate lisinopril purified by means of liquid chromatography-from pilot plant to industrial scale unit, 2005, Industrial & Engineering Chemistry Research, 2005, Vol 44(6), 1860–1867.*

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 sredotočili na selekcijo in optimizacijo gojišč za produkcijo biomase ter farmacevtrsko aktivnih snovi ter možnosti izkoriščanja industrijskih odpadkov. (2) kontrolirano gojenje v bioreaktorju za sterilizirana trdna gojišča (solid-state) iz agroživilske in lesne industrije ter (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 fizikalnih parametrov na tvorbo samih plodišč ter izbrali in optimizirali najboljše substrate. Paralelno s tem so tekle osnovne raziskave produkcije aktivne glivine biomase v smislu gojenja gob na eksperimentalni farmi v Podkorenu.

Dosežki so dokumentirani v prispevkih (članki): *BEROVIČ, Marin, KOŠMERL, Tatjana. Monitoring of potassium hydrogen tartrate stabilization by conductivity measurement. Acta chim. slov.. 2008, 55, 3, str. 535–540, ŠVAGELJ, Mirjan, BEROVIČ, Marin, BOH, Bojana, MENARD, Anja, SIMČIČ, Saša, WRABER-HERZOG, Branka. Solid-state cultivation of Grifola frondosa (Dicks: Fr) S.F. Gray biomass and immunostimulatory effects of fungal intra- and extracellular [beta]-polysaccharides. New biotechnology, 2008, vol. 25, no. 2/3, str. 150–156. GREGORI, Andrej, ŠVAGELJ, Mirjan, PAHOR, Bojan, BEROVIČ, Marin, POHLEVEN, Franc. The use of spent brewery grains for Pleurotus ostreatus cultivation and enzyme production. New biotechnology, 2008, vol. 25, no. 2/3, str. 157–161.*

Dosežki so dokumentirani (v vablenih predavanjih na mednarodnih kongresih): *BEROVIČ, Marin. Solid state and submerged cultivation of Grifola frondosa polysaccharides : [lecture]. V: 17th International ISMS congress : (International Society for Mushroom Science) : Cape Town International Convention Centre, South Africa, 2008. BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Production of antitumor extra and intracellular fungal polysaccharides of Grifola Frondosa by submerged and solid state cultivation : [lecture]. V: 7th European Symposium on Biochemical Engineering, Faro, Portugal, September 7–10, 2008. Book of abstracts : ESBES 7. [S. l.: s. n.], 2008, str. 104. BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Production of pharmaceutically active compounds of Grifola frondosa by solid state and submerged cultivation : [plenary lecture]. V: International conference on technologies and strategic management of suistanable biosystems., 2008, BEROVIČ, Marin. Production of pharmaceutically active compounds of Ganoderma lucidum : 1st International conference on technologies & strategic management of sustainable biosystems, 6–9 july 2008, Perth, Western Australia. 2008; Perth.*

Biokemijsko inženirstvo v vinarstvu: V sklopu raziskav 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.

Dosežek je dokumentiran v prispevkih: *BEROVIČ, Marin, POTOČNIK, Mateja, ŠTRUS, Jasna. The influence of galvanic field on Saccharomyces cerevisiae in grape must fermentation. Vitis, 2008, vol. 47, no. 2, str. 117–122; BEROVIČ, Marin, Invited lecture: New aspects in wine technology and process engineering, National Institute of Wine Technology, Adelaide, 2008, Australia*

Mednarodni patent: Novo anorgansko polnilo za jedro panela in tehnološki postopek izdelave: Patent opisuje razvoj polnila za izolacijske plošče na osnovi ekspandiranega perlita kot tudi tehnološki postopek kontinuirne proizvodnje panelnih plošč z novim polnilom. Poleg tega, da ima razvit produkt zahtevane specifične snovne lastnosti kot so: nizka gostota polnila (od 100 do 160 kg/m^3), dobre mehanske lastnosti, nizko toplotno prevodnost (< 0.045 W/mK), vodoodpornost, hidrofobnost in negorljivost, je tudi biološko neoporečen in okolju prijazen produkt, tehnologija proizvodnje pa je ekonomsko sprejemljiva in okoljevarna. Osnovni tehnološki postopki razvoja novega produkta so mešanje osnovnih surovin, kompaktiranje materiala, mikrovalovno segrevanje, termično tlačna obdelava, hidrofobiranje dobljenih anorganskih plošč polnila in njihovo lepljenje v panele.

Aplikativni rezultati: razvoj novega izdelka, razvoj novega tehnološkega procesa oz. tehnologije, patentna prijava

Učinki aplikativnih rezultatov: razširitev ponudbe novih izdelkov/storitev na trgu, uvajanje novih tehnologij

Vir: *PLAZL, Igor, KAVČIČ, Miha, FRANKO, Urška, BOHOR, Darija. Opis: Novo anorgansko polnilo za jedro panela in tehnološki postopek izdelave: št. prijave P-200600087. Ljubljana: Urad Republike Slovenije za intelektualno lastnino, 11.4.2006.*

RESEARCH PROGRAMME REPORT

PROGRAMME GOALS

Program goals were defined in accordance with the division of main research topics. These are: *Process engineering and modelling*, *Rheology and applications*, *Polymer engineering and technology*, *Bioengineering and biotechnology*, and *Environmental engineering*.

PROCESS ENGINEERING AND MODELLING

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 is used for the description of deposition kinetics of colloidal alkylketene dimer particles on pulp fibers.

Gas holdup data base gained in 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 by the drift-flux model and by 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 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.

The research of nanofiltration in the system with organic solvents to concentrate active pharmaceutical compounds was performed. Comparison between nanofiltration and evaporation was made for the selected solvent and pharmaceutical compound.

Dechlorination of p-chlorophenol was investigated in a microreactor system with bimetallic Pd/Fe catalyst, which enables toxic component removal in situ. The process in continuous-flow microreactor system was only partially efficient at room temperature. By rising the temperature to 60 °C a 90% conversion of p-chlorophenol was obtained at single passage through the reactor. A two-dimensional mathematical model, containing convection, diffusion, and pseudo-first-order catalytic reaction terms, was developed to analyze the experimental data and to forecast the reactor performance.

We investigated the stabilization of PCC dispersions prepared directly in the mother-liquid after the carbonation of (hydrated) lime through the adsorption of a commercial sodium polyacrylate dispersant. The results demonstrated that the composition of the mother-liquid, particularly the Ca^{2+} activity, strongly influenced virtually all the processes pertinent to dispersion stabilization, from the initial charging of the $CaCO_3$ surface in base PCC dispersions, to the surface charge regulation and dispersion stabilization efficiency of the polyacrylate dispersing agent. The increasing prominence of the counterion condensation affected in Ca^{2+} -rich solutions limits the conditions conductive to the surface charge regulation through dispersant adsorption to an optimum pH range of about 8–11. Furthermore, the dispersion stability analysis, based on traditional DLVO theory of colloid stability, together with experimental evidence in

the form of particle size distribution analyses, also indicated that optimum stability conditions for such PCC dispersions were established with small dispersant doses (0.25–0.5% per dry weight) in the pH range of about 9–11.

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. These bitumens are most frequently used in Slovenia for the production of asphalt mixtures for wearing and wearing-close courses. The experimental work was carried out by using standard test methods and rheological characterization. Part of the filler in bituminous mortars was replaced with HL, the amount of HL varying from 0 to 20 wt.%. All the samples were examined before and after forced temperature ageing and after bituminous binder extraction (by trichloro-ethylene).

The pressure drop, which resulted from polyamide 6 flow through industrial spinnerets and wire-mesh filters, was examined as a possible parameter for improving spinning process constancy by experimental techniques and numerical approach. All the necessary basic material information was obtained to fit the data with the purely viscous Cross model and the viscoelastic Kaye, Bernstein, Kearsley, Zappas (K-BKZ) model. The results, with respect to the spinneret geometry, led to the conclusion that the numerical simulations gave satisfactory predictions even for experimental data coming from complex systems such as spinning plants, as long as extensional properties were accounted for by the model. On the contrary, pressure drop predictions obtained from the Cross model underestimated the pilot plant values by approximately 20% because of the inability of the model to consider the extensional component of the flow.

One of the objects 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 with a Rushton turbine: Water-CMC solutions at w = 0.5% and w = 1% mass fraction and compressed air were used. The apparent viscosity, enabling 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 and was in good agreement with the results found in literature.

POLYMER ENGINEERING AND TECHNOLOGY

Developments in these fields request 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 following programme goals have been achieved: the kinetics of vulcanization process and heat transfer during vulcanization process for different rubber blends were studied and the processes were described by mathematical modelling. The viscoelastic behavior of elastomeric systems in a wide range of temperatures and frequencies was determined and modeled, nanocomposites were prepared from elastomers representing the polymer matrix and montmorillonite treated with modifier molecules as a filler. They were carefully characterized and their properties were studied, the unsaturated polyurethane (PU) was synthesized, characterized, and used in different rubber matrixes, i.e. (natural rubber (NR), butadiene

rubber (BR), and NR/BR blend) to improve their properties. BR, SBR (styrene-butadiene rubber), NR rubbers and their blends were investigated to estimate the degree of miscibility of the components in the blends, a testing apparatus for testing automotive timing belt abrasion resistance was developed, the kinetics of phenol-formaldehyde and melamine-formaldehyde resins synthesis and curing were studied and modelled, a technology for melamine foam production was developed, the kinetics of diallyl terephthalate free radical polymerization together with monomer in polymer diffusion was studied and modelled; the synthesis of water-based polyurethane dispersions was studied, and polyurethane chemical structure and polymer film properties were correlated, a semibatch emulsion polymerization process for water-based acrylic-polyurethane hybrid emulsions production was developed and studied, the kinetics of emulsion polymerization of acrylic monomers in the presence of polyurethane seeds was investigated, the properties water-based acrylic-polyurethane hybrid emulsions and their polymer films were studied and designed, the suspension polymerization of acrylic monomers was studied, synthesis and product properties of acrylic microsphere pressure sensitive adhesives were optimized, the synthesis of one-component urethane adhesives was studied. On the basis of previous experimental work the ability of designing adhesive properties was developed, a new one-component urethane adhesive was developed, and a new in-line injection molding machine mounted measurement system was developed.

BIOCHEMICAL ENGINEERING AND BIOTECHNOLOGY

Based on our previous studies on the influence of bioprocess parameters on fungal morphology and estimation of kinetic parameters of progesterone biotransformation in the presence of β-cyclodextrin, a continuous process of progesterone 11α-hydroxylation with Rhizopus nigricans pellets at a laboratory-scale stirred-tank bioreactor was developed. 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 enables very efficient mass transfer and low consumption of chemicals.

The main goal of our recent studies was to implement the microreactor technology in biocatalytic processes and to define the basic transport phenomena and fluid flow dynamics within microchannels by the application of modern modelling. Microstructured devices have demonstrated several advantages in (bio)chemical processes, especially due to the very large surface-area-to-volume ratio, connected with very effective heat and mass transfer, easier control of process parameters and new production concepts by numbering-up instead of scaling-up to increase the production capacity.

Research on pharmaceutically active compounds of *Grifola frondosa*: Research of pharmaceutically active compounds of *Grifola frondosa* went in three main directions: (1) Submerged cultivation on liquid substrate in stirred tank reactor was optimized in relation to 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 agriculture industry wastes on experimental pilot mushroom farm was carried out. The goal of this research was to optimize various fermentation substrates for active biomass and production. Protocols for effective isolation and purification of external and internal fungal polysaccharides were developed.

Activated fungal strain G3 was applied in all the experiments in submerged cultivation in shaken cultures and stirred tank reactors, as well as in solid state cultivation on corn straw substrate. Parallel to this the research in pilot experiments on experimental farming solid substrates, based on

wood and agriculture industry wastes were studied. From the active fungal biomass of all three kinds of cultivation, we isolated fungal extra- and intracellular polysaccharides.

Biochemical engineering in wine technology: In searching for new pathways for high glicerol production in wine technology a new method based on heat shock of *Saccharomyces cerevisiae* suspension was developed. High glicerol concentration up to 12 g l–1 (100% incerasement) was developed at increasement of ethanol for 10% at only slight increasement of volatile acids. This method represents a new and original technology suitable for large scale production too.

ENVIRONMENTAL ENGINEERING

Bioremediation: The aim of this research was to prepare a mixture of ligninolytic enzymes for decolourization of synthetic dyes, usuallly present in waste waters from textile industry. Decolorization of azo dye Reactive Orange 16 by immobilized cultures of *Irpex lacteus* was studied in three different bioreactor systems at a laboratory scale. The highest dye decolorization efficiency was observed in a trickle bed reactor. It was found that extracellular, as well as mycelium-associated activities, contribute to the decolorization process. It was also found out that the decolourization rate had the shifting reaction order from 0.7 at low dye concentration to 1.0 at higher dye concentrations.

The research was continued with white rot fungus *Ceriporiopsis subvermispora*, known for the production of laccase (Lac) and manganese peroxidase (MnP) for the application in biopulping. The procedure for the enzyme production in stationary cultures was optimized with regard to the type of sugar as a source ofcarbon, type of wood as an inductor and immobilization support material as well as additional nitrogen supply. By varying the culture conditions, production media with the excess of Lac activity, equivalence of both activities and excess of MnP activity were prepared and further used to decolorize three structurally different dyes: RBBR, CuP and RO16. It was found out that specific enzyme activities better decolourize dyes with a specific chemical structure.

The enzyme production with white rot fungus *Dichomitus squalens* in static cultures was optimized with regard to the type of carbon and nitrogen sources, and type of support material. Beech wood and straw were the best inducers and immobilization supports; fructose better stimulated enzyme activities than other sugars, while additional nitrogen increased the enzyme activities. Three structurally different dyes were used to test the prepared enzyme mixtures. After 10 hours of decolourization process, the percent of degradation was 62% for RBBR, 50% for Copper(II)phthalocyanine, and 19% for RO16.

RESEARCH TOPICS

Process engineering and modelling:

- 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 modelling of the 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
– 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 modelling
– Heat transfer investigations during vulcanization process for different rubber blends and modelling
– Synthesis, preparation and characterization of nanocomposite materials
– Testing of rubber and rubber composites
– Synthesis, characterization, modelling 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 the 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

Acrylic-polyurethane hybrid emulsions for coatings: synthesis, characterization and use: The research activities included basic and applied studies. The goal of this project was to develop a new, environmental friendly, water based, hybrid coating for metal surfaces which would demonstrate the advantages of the AC and PU components. Several other research and development achievements have been gained from this work. The kinetics of AC monomer (methyl methacrylate (MMA)) polymerization in the presence of different PU dispersions of different compositions and properties was investigated. AC-PU hybrid emulsions were prepared by semibatch emulsion polymerization. The PU rigidity was controlled by varying the polyol chemical structure, polyol molecular weight and by adding butanediol. We studied the effect of the use of different PU seed particles on the rate of polymerization, particle size and distribution, number of particles, and the average number of radicals per particle. The monomer feed rate was varied in order to study its influence on the process. It was observed that the PU particles that had been prepared with a higher polyol molecular weight, swelled better with MMA before the monomer-starved conditions occurred. There seemed to be no significant discrepancies between the series with different PU seeds in the monomer-starved conditions. The overall conversion depended on the monomer addition rate, and the polymerization rate acquired a constant value, which was comparable to the value of monomer addition rate. The instantaneous conversion increased slightly. The average particle size increased, and the total particle number in the reactor was constant and similar to the number of PU particles in the initial charge. The average number of radicals per particle increased. The semibatch emulsion polymerization of MMA in the presence of PU particles studied was better, compared to the system with fixed radical concentration. It was observed that the addition of butylacrylate (BA) monomer in the adhesive composition improved its mechanical properties which are required for achieving a desired coating performance. Therefore, in the subsequent study the semibatch emulsion copolymerization of MMA and BA in the presence of PU dispersions was investigated. In further studies AC-PU hybrid emulsions were prepared by the use of MMA and BA. The effect of the use of different PU seed particles and the effect of different weight ratio between MMA and BA on the emulsion properties, microphase structure, and mechanical properties of hybrid films were studied. On the basis of this research the AC-PU hybrid emulsion composition, which gives required coating properties, was established. The results of research work are of major importance for Slovenian coating industry. Pilot plant researches are in progress. From the scientific point of view the significance of our work has been confirmed by several citations (21 in the last four years). The results were presented at several conferences, technology networks and platforms, and published in scientific journals: *ŠEBENIK, Urška, KRAJNC, Matjaž. Seeded semibatch emulsion copolymerization of methyl methacrylate and butyl acrylate using polyurethane dispersion : effect of soft segment length on kinetics. Colloids surf., A Physicochem. eng. asp., 2004, Vol. 233, No. 1/3, pp. 51–62.*, *ŠEBENIK, Urška, KRAJNC, Matjaž. Semibatch emulsion polymerization of methyl methacrylate using different polyurethane particles. J. polym. sci., Part A, Polym. chem., 2005, Vol. 43, No. 4, pp. 844–858.* and *ŠEBENIK, Urška, KRAJNC, Matjaž. Properties of acrylic-polyurethane hybrid emulsions synthesized by the semibatch emulsion copolymerization of acrylates using different polyurethane particles. J. polym. sci., Part A, Polym. chem., 2005, Vol. 43, No. 18, pp. 4050–4069.*

Kinetic and heat transfer investigations during vulcanization process for different rubber blends and modelling: The vulcanization kinetics of conventional blend types was studied where polybutadiene (BR) and polyisoprene (NR) rubber was chosen as an example. In the case of vulcanization of NR and BR compound kinetic parameters were obtained by using regression analysis of the developed model and based on experimental data from differential dynamic calorimetry, and dynamic mechanical analysis measurements. By considering the variation of heat transfer dur-

ing 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 relatively low rate of reversion was observed as well. Heat transfer is often very important in many 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 the cross-linking kinetics. Heat transfer in several elastomers was studied on a pilot scale mold utilizing various expressions for description of temperature dependent elastomer densities, heat capacities and thermal conductivities, which were applied in the governing heat equation. The latter was solved by the means of quasi-exact and explicit finite difference algorithms. Molding experiments were performed for natural rubber, polybutadiene, hydrogenated butadiene-acrylonitrile copolymer, polychloroprene and polyisoprene. 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. The research results support fundamental undersatnding of a complex reaction scheme and heat transfer during vulcanization. The developed model enables several optimizations of production processes. The production time of vulcanized products was lowered by 40%. The results of the work were presented at international conferences, technology networks and platforms, and were published in scientific articles: *LIKOZAR, Blaž, KRAJNC, Matjaž. Temperature dependent dynamic mechanical properties of hydrogenated nitrile butadiene rubber and the effect of peroxide cross-linkers. E-polymers., 2007, No. 131, pp. 1–20.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Kinetic and heat transfer modelling 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, pp. 293–30,.* and *A.01 – LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Modelling of dynamic mechanical properties of vulcanized fluoroelastomer. Polym. eng. sci., 2007, Vol. 47, No. 12, pp. 2085–2094.*

Dechlorination of p-chlorophenol in a single-pass, continuous-flow microreactor system: Dechlorination of p-chlorophenol was investigated in a single-pass, continuous-flow microreactor system made of two parallel palladized iron plates. The plates formed a 27 mm wide, 70 mm long, and 0.2 mm high microscale channel. The bimetallic catalyst was prepared by electroless deposition of Pd on the reactor plate surfaces. The experiments were performed under steady-state conditions at different temperatures between 293 and 333 K and at a variety of flow conditions in the range from 1.5×10^{-9} to 1×10^{-8} m^3/s. A two-dimensional mathematical model, containing convection, diffusion, and pseudo-first-order catalytic reaction terms, was developed to analyze the experimental data and to forecast the reactor performance. Depending on the prevailing kinetic and convection/diffusion phenomena, the developed model can be reduced to an ideal plug-flow model or can depict reactor performance that is close, or even worse than the performance of an ideal mixed-flow reactor. Under operating conditions typical to this study, the model and the experimental data indicate plug-flow behavior of the microreactor. Analysis of the obtained chemical kinetic rate constants provides an estimate of the activation energy for this reaction (E_a = 48.43 +/– 6.13 kJ/mol), which remains unchanged despite the observed deactivation of the catalyst. The deactivation of the catalyst is caused by reversible catalyst passivity, and it is modelled by second-order kinetics. Analysis of the experimental data shows that the observed deactivation influences only the pre-exponential factor in the Arrhenius law for the investigated reaction. The research results were presented at various conferences and published in *JOVANOVIĆ, Goran, ŽNIDARŠIČ PLAZL, Polona, SAKRITTICHAI, Ploenpun, AL-KHALDI, Khaled. Dechlorination of p-chlorophenol in microreactor with bimetallic Pd/Fe catalyst. Ind. Eng. Chem. Res., 2005, 44 (14), 5099–5106.*

Steroid extraction in a microchannel system: A continuous ethyl acetate extraction of progesterone and 11 alpha-hydroxyprogesterone, the reactant and the product of the biotransformation step

involved in corticosteroid production, was studied 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 with considerations to 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 11 alpha-hydroxylation of progesterone by Rhizopus nigricans in the form of pellets. The results of research work were presented at inertnational conference (invited lecture – I. Plazl, Studies at the microreactor scale, Symbiosis: science, industry & society, Barcelona, 2007) and published in *ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor. Steroid extraction in a microchannel system: mathematical modelling and experiments. Lab chip, 2007, 7 (7), 883–889.*

Suspension polymerization for the synthesis of microsphere pressure sensitive adhesives: The influence of polymer molecular weight and crosslinking reactions on the adhesion properties of (PSA) was investigated. Inherent polymer properties, such as copolymer composition, polymer microstructure and molecular weight are the most important factors affecting adhesion properties of the microsphere PSA directly, as well as indirectly through their influence on the physical properties (e.g., T_g) and consequently also rheological properties of the polymer. An important problem related to 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 becomes complicated by intermolecular and intramolecular (backbiting) transfer to polymer and this process leads to the formation of gel phase in the adhesive. In addition to the intramolecular transfer to polymer, the amount of both, crosslinked polymer molecules, as well as highly entangled and coiled polymer molecules contribute to the formation of gel phase in the adhesive. Molecular weight of the adhesive was modified by introducing a chain transfer agent (n-dodecylmercaptane), and the crosslinking reactions were induced by adding either di- or triacrylate acrylic monomers (butanediol diacrylate and trimethylolpropane triacrylate). The results of our study show that all adhesive properties strongly depend on added modifiers even in low concentrations. 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 montmorillonite (MMT) clays. By this procedure we significantly improved shear properties of the microsphere PSA's. The results of research work were used to optimize the production process of PSA adhesives and were published in: *KAJTNA, Jernej, KRAJNC, Matjaž, GOLOB, Janvit. The role of components in waterbased microsphere acrylic PSA adhesive properties. Macromol. symp., 2006, vol. 243, no. 1, str. 132–146.*, *KAJTNA, Jernej, LIKOZAR, Blaž, GOLOB, Janvit, KRAJNC, Matjaž. The influence of the polymerization on properties of an ethylacrylate/2-ethyl hexylacrylate pressure-sensitive adhesive suspension. Int. j. adhes. adhes., 2008, Vol. 28, No. 7, pp. 382–390.* and *KAJTNA, Jernej, ŠEBENIK, Urška, KRAJNC, Matjaž, GOLOB, Janvit. IR drying of water-based acrylic PSA adhesives. Dry. technol., 2008, Vol. 26, No. 3, pp. 323–333.*

OTHER RELEVANT ACHIEVEMENTS

Development of water-based polyurethane dispersions, acrylic-polyurethane hybrid emulsions, and research and technology development of water-based coatings for metal substrates: New, environmentally friendly products of high performance and new technologies for the

Slovenian paint industry were developed: (i) a water-based polyurethane dispersion, (ii) a water-based acrylic-polyurethane (AC-PU) hybrid emulsion, (iii) a water-based, heavy-duty coating for metal surfaces with the use of AC-PU adhesive. As a result of the project work two postgraduate students, employed by Helios d.d., obtained a master's degree.

Applicable results: development of new products, development of new technologies, new practical knowledge, information and skills, new scientific knowledge.

Effects of applicable results: development of undergraduate education, development of postgraduate education, expanding the supply of new products/services to the market, greater competitive ability, improvement of educational structure of the employees, and preserving the environment and sustainable development

The achievement was presented at several international conferences: *ŠEBENIK, Urška, KRAJNC, Matjaž. Semibatch emulsion polymerization of methyl methacrylate using different polyurethane seed particles, 7th world congress of chemical engineering, Incorporating the 5th European congress of chemical engineering, SECC, Glasgow, Scotland, 10–14 July 2005., ŠEBENIK, Urška, KRAJNC, Matjaž. Rheological properties of acrylic-polyurethane hybrid emulsions synthesized by semibatch emulsion polymerization of acrylates using different polyurethane seed particles, 2nd Annual European Rheology Conference, April 21–23, 2005, Grenoble, France., ŠEBENIK, Urška, KRAJNC, Matjaž. Kinetics of methyl methacrylate polymerization in polyurethane dispersions, 9th Austrian Polymer Meeting, March 26–28 2008, Graz, Austria*. Two master thesis: *GLAVAČ, Alenka. Sinteza in karakterizacija poliuretanskih vodnih disperzij : magistrsko delo. Ljubljana, 2004.* and *VEZOČNIK, Borut. Razvoj in tehnologija priprave poliuretansko-akrilatnega pokrivnega premaza na vodni osnovi za zaščito kovin : magistrsko delo. Ljubljana, 2006.*

Improvement of products and production processes for rubber industry: In cooperation with Goodyear Engineered Products Europe the following results were achieved: (i) the required time and energy for products vulcanization was significantly shortened, (ii) the rubber blend was modified and improved, (iii) a testing apparatus for automotive timing belt abrasion resistance was developed. This is a fast-test and gives results in a very short time. (iv) the mechanical properties and abrasion resistance of automotive timing belt were improved.

Applicable results: product improvement, improvement of production methods, instruments and processes

Effects of applicable results: development of undergraduate education, development of postgraduate education, expanding the supply of new products/services to the market, greater competitive ability, increase of educational structure of employees, technological expansion/modernisation of activities, and introduction of new technologies.

The achievements are documented in several phase reports for the Goodyear E.P.E, which are listed in the COBISS database. The results were presented at several international conferences: *LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Hydrogenated acrylonitrile butadiene elastomer/coagent nanocomposites : [oral contribution], European polymer congress [also] epf, 2–6 july, 2007, Congress centre Bernardin, Portorož, Slovenia*., *ŠEBENIK, Urška, ZUPANČIČ-VALANT, Andreja, MESEC, Aleš, KRAJNC, Matjaž. Investigation of rubber-rubber blends miscibility by RPA and modulated-temperature DSC, 2nd Annual European Rheology Conference, April 21–23, 2005, Grenoble, France.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Sulfur vulcanization of various BR/NR blends with TBBS and TBSI accelerators : heat transfer, kinetics and rheology, Polymer Reaction Engineering VI, May 21–26, 2006, Hali-*

fax, Nova Scotia, Canada., *LIKOZAR, Blaž, KRAJNC, Matjaž. Kinetic modelling of peroxide vulcanization of hydrogenated nitrile butadiene rubber, Hangzhou International Polymer Forum, Hangzhou, China, May 13–17, 2007.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Viscoelastic behavior of hydrogenated nitrile butadiene rubber and the effect of coagents, Hangzhou International Polymer Forum, Hangzhou, China, May 13–17, 2007.*, *LIKOZAR, Blaž, ŠEBENIK, Urška, KRAJNC, Matjaž. Dynamic mechanical properties of hydrogenated nitrile butadiene rubber at various temperatures and their modelling, European polymer congress [also] epf, 2–6 july, 2007, Congress centre Bernardin, Portorož, Slovenia.*, *LIKOZAR, Blaž, KRAJNC, Matjaž. Determination of thermophysical properties of various elastomers, 9th Austrian Polymer Meeting, March 26–28 2008, Graz, Austria.*

Development of PSA adhesives: In cooperation with the company Aero, d.d, we developed and optimized new acrylic waterbased PSA adhesives. As a result of this project a postgraduate student employed by Aero, d.d., obtained a PhD degree.

Applicable results: development of new products, development of new technologies, new practical knowledge, information and skills, new scientific knowledge.

Effects of applicable results: development of undergraduate education, development of postgraduate education, expanding the supply of new products/services to the market, greater competitive ability, increase of educational structure of employees, and preserving the environment and sustainable development

The achievements were presented at several international conferences: *KAJTNA, Jernej, KRAJNC, Matjaž, GOLOB, Janvit. Microsphere acrylic pressure sensitive adhesives : the influence of process and chemical parameters on adhesion properties : [oral contribution]: European polymer congress, 2–6 july, 2007, Congress centre Bernardin, Portorož, Slovenia. Ljubljana, 2007.*, *KAJTNA, Jernej, GOLOB, Janvit, KRAJNC, Matjaž. The role of components in waterbased microsphere acrylic PSA adhesive properties: Polymer Reaction Engineering VI, May 21–26, 2006, Halifax, Nova Scotia, Canada. Program : ECI : Engineering Conferences International., 2006.*, *KAJTNA, Jernej, KRAJNC, Matjaž, GOLOB, Janvit. The effect of gel phase on adhesion properties of microsphere suspension based acrylic pressure sensitive adhesives : Hangzhou International Polymer Forum, Hangzhou, China, May 13–17, 2007. Advanced materials and reaction engineering., 2007.*, *KAJTNA, Jernej, ŠEBENIK, Urška, KRAJNC, Matjaž. Microsphere pressure sensitive adhesives : acrylic polymer/montmorillonite clay nanocomposite materials : 9th Austrian Polymer Meeting, March 26–28 2008, Graz, Austria, 2008.* and in doctorate thesis: *KAJTNA, Jernej. Suspension polymerization and drying of microspheric acrylic adhesives: doctoral thesis. Ljubljana, 2008.*

Research on pharmaceutically active compounds of *Grifola frondosa*: 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 agriculture industry wastes on experimental pilot mushroom farm. The goal of this research was to optimize various fermentation substrates for active biomass and production. Protocols for effective isolation and purification of external and internal fungal polisaccharides were developed. Paralel with this the research in pilot experiments on experimental farming solid substrates based on wood and agriculture industry wastes were studied.

The achievements are documented in: *BEROVIČ, Marin, KOŠMERL, Tatjana. Monitoring of potassium hydrogen tartrate stabilization by conductivity measurement. Acta chim. slov.*

2008, No.55, 3, pp. 535–540, ŠVAGELJ, Mirjan, BEROVIČ, Marin, BOH, Bojana, MENARD, Anja, SIMČIČ, Saša, WRABER-HERZOG, Branka. Solid-state cultivation of Grifola frondosa (Dicks: Fr) S.F. Gray biomass and immunostimulatory effects of fungal intra- and extracellular [beta]-polysaccharides. New biotechnology, 2008, Vol. 25, No. 2/3, pp. 150–156. GREGORI, Andrej, ŠVAGELJ, Mirjan, PAHOR, Bojan, BEROVIČ, Marin, POHLEVEN, Franc. The use of spent brewery grains for Pleurotus ostreatus cultivation and enzyme production. New biotechnology, 2008, vol. 25, no. 2/3, pp. 157–161.

The achievements were presented at several international conferences as invited lectures: *BEROVIČ, Marin. Solid state and submerged cultivation of Grifola frondosa polysaccharides : [lecture]. V: 17th International ISMS congress : (International Society for Mushroom Science) : Cape Town International Convention Centre, South Africa, 2008. BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Production of antitumor extra and intracellular fungal polysaccharides of Grifola Frondosa by submerged and solid state cultivation : [lecture]. V: 7th European Symposium on Biochemical Engineering, Faro, Portugal, September 7–10, 2008. Book of abstracts : ESBES 7. [S. l.: s. n.], 2008, pp. 104. BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Production of pharmaceutically active compounds of Grifola frondosa by solid state and submerged cultivation : [plenary lecture]. V: International conference on technologies and strategic management of suistanable biosystems., 2008, BEROVIČ, Marin. Production of pharmaceutically active compounds of Ganoderma lucidum : 1st International conference on technologies & strategic management of sustainable biosystems, 6–9 July 2008, Perth, Western Australia. 2008; Perth.*

Biochemical engineering in wine technology: In searching for new pathways for high glicerol production in wine technology a new method, based on heat shock of *Saccharomyces cerevisiae* suspension was developed. High glicerol concentration up to 12 g l–1 (100% incerasement) was developed at increasement of ethanol by 10% at only slightl increasement of volatile acids. This method represents a new and original technology suitable for large scale production.

The achievement is documented in: *BEROVIČ, Marin, POTOČNIK, Mateja, ŠTRUS, Jasna. The influence of galvanic field on Saccharomyces cerevisiae in grape must fermentation. Vitis, 2008, Vol. 47, No. 2, pp. 117–122; BEROVIČ, Marin, Invited lecture: New aspects in wine technology and process engineering, National Institute of Wine Technology, Adelaide, 2008, Australia.*

Concentration of Lisinopril by reverse osmosis: Lisinopril is an active pharmaceutical ingredient produced through a stepwise chemical synthesis. After purification by means of low-pressure liquid chromatography it has to be concentrated. For this purpose, the reverse osmosis was tested under various process conditions on a pilot-scale unit. These data were used for capital and operating cost estimation for the industrial reverse osmosis unit and evaporator, as well as for conceptual design and installation of the industrial scale reverse osmosis unit. The capital cost estimate agreed reasonably well with the purchased unit and is significantly lower compared to a single-stage batch vacuum evaporator. The validation results of the full-scale unit and its trouble-free operation prove that the decision for reverse osmosis is economically justified and that the scale-up has been technically successful.

Applicable results: implementation of existing technologies in practice, improvement of existing production process.

Effects of applicable results: development of undergraduate education, development of postgraduate education, technological expansion/modernisation of activities, and introduction of new technologies.

The results are documented in: *D. Senica, J. Ržen, M. Uštar, P. Drnovšek, S. Kogej, A. Pavko: Reverse osmosis to concentrate lisinopril purified by means of liquid chromatography-from pilot plant to industrial scale unit, 2005, Industrial & Engineering Chemistry Research, 2005, Vol. 44(6), 1860–1867.*

Patent: New inorganic core for sandwich panels and production technology: The patent describes the development of new core for sandwich panels based on expanded perlite. A lightweight building material is composed of expanded perlite as an additive and a bonding inorganic agent. Non-flammable isolated plates of low density (from 100 to 160 kg/m^3) and heat conductivity <0.045 W/mK) with appropriate mechanical properties are biologically and environmentally safe products. The proposed technology production is based mainly on mixing, compression, microwave heating, thermal treatment, and water-repellency.

Applicable results: development of new products, development of new technologies, patent application

Effects of applicable results: Expanding the supply of new products/services to the market, introduction of new technologies.

Source: *PLAZL, I., Kavčič, M., Franko, U., Bahor, D. New anorganic core for sandwich panels and technology of production. Patent reg. P-200600087, 2006.*

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 2008
CHAIRS IN 2008

KATEDRA ZA ANALIZNO KEMIJO
CHAIR OF ANALYTICAL CHEMISTRY

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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	2006–2010	doktorski študij / *PhD*
Gregor Arh	M. Veber	2006–2010	doktorski študij / *PhD*
Andrej Ščavničar	M. Pompe	2007–2012	doktorski študij / *PhD*
Alenka Možir	M. Strlič	2008–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

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

Analizna kemija */ Analytical Chemistry* – VS

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

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

Avtomatizirana analiza */ Automated Analysis* – UN

Instrumentalna analiza */ Instrumental Analysis* – UN

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

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

Kemija okolja / *Environmental Chemistry* – UN

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

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

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 – UN in VS
Analizna kemija / *Analytical Chemistry* PEF – UN
Kemija okolja / *Environmental Chemistry* PEF – UN

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

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

– E. Menart, Prešernova nagrada FKKT za leto 2008 (mentor M. Strlič) / *The Faculty Pešeren Award for 2008*

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
– Atomski absorpcijski spektrometer Perkin Elmer 1100B / *AAS Spectrometer Perkin Elmer 1100B*
– Atomski absorpcijski spektrometer PerkinElmer AAnalyst 600 / *AAS Spectrometer Perkin Elmer AAnalyst 600*
– Atomski absorpcijski spektrometer Varian AA 240 / *AA Spectrometer Varian AA 240*
– 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

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
LLP-LDV-TOI-2008-SI-15	*Hands-On Approach to Analytical Chemistry for Vocational Schools (II)* 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 – 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 – Hrvaška *Slovenia – Croatia*	Razvoj mikrosenzorjev z nanostrukturiranimi katalizatorji za elektrokemijsko detekcijo vodikovega peroksida / *Development of Nanostructured Catalyst-Based Sensors for Electrochemical Detection of Hydrogen Peroxide* Nosilec / *Principal Researcher*: B. Pihlar
Slovenija – Hrvaška *Slovenia – Croatia*	Uporaba metod diskretne matematike za identifikacijo kemijsko aktivnih struktur / *Application of Discrete Mathematics for the Identification of Active Chemical Structures* Nosilec / *Principal Researcher*: M. Pompe
Slovenija – Turčija *Slovenia – Turkey*	Sistem nadzora in sledljivosti biogenih aminov in nitrozamina v tradicionalnih ribjih produktih / *Systems of Control and Traceability of Biogenetic Amines and Nitrosamines in Traditional Fish Products* Nosilec / *Principal Researcher*: M. Pompe

BIBLIOGRAFIJA 2008 / REFERENCES 2008

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

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AL2. LICHTBLAU, Dirk Andreas, STRLIČ, Matija, TRAFELA, Tanja, KOLAR, Jana, ANDERS, Manfred. Determination of mechanical properties of historical paper based on NIR spectroscopy and chemometrics : a new instrument. *Appl. phys., A, Mater. sci. process. (Print)*, 2008, vol. 92, no. 1, str. 191–195, graf. prikazi. [COBISS.SI-ID 29804549]

AL3. TURŠIČ, Janja, RADIČ, Helena, KOVAČEVIČ, Miroslav, VEBER, Marjan. Determination of selected trace elements in airborne aerosol particles using different sample preparation = Določevanje nekaterih elementov v sledovih v atmosferskih delcih. *Arh. hig. rada toksikol.*, 2008, vol. 59, no. 2, str. 111–116, graf. prikazi. [COBISS.SI-ID 29941253]

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AL6. PROSEN, Helena, KOČAR, Drago. Different sample preparation methods combined with LC-MS/MS and LC-UV for determination of some furocoumarin compounds in the products containing citruses. *Flavour fragr. j.*. [Print ed.], 2008, vol. 23, no. 4, str. 263–271. [COBISS.SI-ID 29682437],

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AL24. GABOR, Boštjan, URBAS, Lidija, BARUT, Miloš, BRNE, Peter, PLEVČAK, Sašo, ČERK-PETRIČ, Tatjana, ZUPANČIČ-KRALJ, Lucija, ŠTRANCAR, Aleš. Kromatografska predpriprava krvne plazme za analizo proteoma z uporabo CIM monolitnih kolon = Chromatographic fractionation of the human plasma with the use of CIM monolithic columns for the proteome analysis. V: RASPOR, Peter (ur.), JAMNIK, Polona (ur.). Posvetovanje Pomen biotehnologije in mikrobiologije za prihodnost, 31. januar in 1. februar 2008, Ljubljana. *Proteomika*, (Pomen biotehnologije in mikrobiologije za prihodnost, 05). Ljubljana: Biotehniška fakulteta, Oddelek za živilstvo, 2008, str. 85–96. [COBISS.SI-ID 3403384]

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AL32. WEINGERL, Vesna, STRLIČ, Matija, KOČAR, Drago. Primerjava metod za določanje fenolnih antioksidantov v vinu = Comparison of analytical methods for determination of phenolic antioxidants in wines. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, 1–6 str. [COBISS.SI-ID 2699820]

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AL34. MOZETIČ, Branka, FAJT, Nikita, KOMEL, Erika, KOČAR, Drago, STRLIČ, Matija, TREBŠE, Polonca. Določanje vsebnosti fenolov v slivah in češnjah = Determination of plums and sweet cherry phenols. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, str. 1–8. [COBISS.SI-ID 959227]

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

AL35. STRLIČ, Matija, ŠELIH, Vid Simon, KOLAR, Jana. Analytical methods based on laser ablation sampling. V: SCHREINER, Manfred (ur.), STRLIČ, Matija (ur.), SALIMBENI, Renzo (ur.). *Handbook of the use of lasers in conservation and conservation science*. Brussels: COST office, 2008, poglavje 4.5. [COBISS.SI-ID 29199365]

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

AL36. PIHLAR, Boris. *Osnove analizne kemije: zapiski predavanj*. (Ponatis). Ljubljana: Fakulteta za kemijo in kemijsko tehnologijo, 2008–. Zv. <1>, ilustr. ISBN 978-961-6286-42-8. ISBN 978-961-6286-43-5. [COBISS.SI-ID 235267840]

PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

AL37. KOČAR, Drago. *Determination of antioxidants and biogenic amines by LC-MS-MS : [Karadeniz Technical University, Trabzon, Turkey, 3. 10. 2008]*. Trabzon, 2008. [COBISS.SI-ID 29862149]

AL38. POMPE, Matevž. *Experimental and theoretical research on structure-property correlations in analytical and environmental chemistry : [Department of Physics, Texas Southern University, February 7th, 2008, Houston, Texas]*. Houston, 2008. [COBISS.SI-ID 29264645]

AL39. GROS, Nataša. Small-scale low-cost analytical instruments: new teaching oppurtunities for schools : [University of Gdansk, Faculty of Chemistry, Gdansk, Poland, February 7th, 2008]. Gdansk, 2008. [COBISS.SI-ID 29874181]

UREDNIK / EDITOR

AL40. PROSEN, Helena (ur.). 15th Young Investigators' Seminar on Analytical Chemistry, Ljubljana, Slovenia, July 2–5, 2008. *Book of abstracts*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2008. 143 str., ilustr. ISBN 978-961-6286-96-1. [COBISS.SI-ID 239668224]

AL41. KOLAR, Jana (ur.), STRLIČ, Matija (ur.). *Cultural heritage meet practice : book of abstracts : conference preprints*. Ljubljana: Narodna in univerzitetna knjižnica, 2008. ISBN 978-961-6551-25-0. [COBISS.SI-ID 2230660]

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AL43. STRLIČ, Matija (ur.), KOLAR, Jana (ur.). *Durability of paper and writing 2 : book of abstracts : 2nd international symposium and workshops, Ljubljana, Slovenia, July 7–9, 2008*. Ljubljana: Faculty of Chemistry and Chemical Technology, 2008. 100 str., ilustr. ISBN 978-961-6286-97-8. [COBISS.SI-ID 239671296]

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AL46. *Acta chimica slovenica*. Strlič, Matija (urednik 2003–, gostujoči urednik 2007), Pihlar, Boris (član uredniškega odbora 1998–), Veber, Marjan (član uredniškega odbora 1998–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [COBISS.SI-ID 14086149]

AL47. *E-preservation science*. Strlič, Matija (urednik 2004–), Kolar, Jana (urednik 2004–). Ivančna Gorica: Morana RTD, 2004–. ISSN 1581-9280. [COBISS.SI-ID 214150912]

AL48. *Kvarkadabra*. Kolar, Jana (član uredniškega odbora 2005–). Ljubljana: Kvarkadabra, 1999–. ISSN 1580-3937. [COBISS.SI-ID 107906048]

AL49. *Restaurator*. Kolar, Jana (urednik 2004–). Copenhagen: Munksgaard, 1969–. ISSN 0034-5806. [COBISS.SI-ID 5531146]

KATEDRA ZA ANORGANSKO KEMIJO
CHAIR OF INORGANIC CHEMISTRY

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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 Medveščček	A. Meden	2003–2010	doktorski študij / *PhD*
Katarina Stare (Demšar)	A. Meden	2006–2010	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*
Rosana Hudej	I. Turel	2008–2012	doktorski študij / *PhD*
Jakob Kljun	I. Leban	2008–2012	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* – VS
Splošna kemija / *General Chemistry* – UN
Kemija in kemijska tehnologija / *Chemistry and Chemical Technology* – VS
Anorganska kemija / *Inorganic Chemistry* – UN in VS
Anorganska kemija II / *Inorganic Chemistry II* – UN
Bioanorganska kemija / *Bioinorganic Chemistry* – UN
Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UN
Izbrana poglavja iz anorganske kemije / *Selected Topics in Inorganic Chemistry* – UN
Kemija kompleksov / *Chemistry of Complexes* – UN
Kristalna kemija / *Crystal Chemistry* – UN
Metodika anorganskih eksperimentov / *Methodology of Inorganic Experiments* – UN

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 – UN
Kemija / *Chemistry* NTF – UN in VS
Kemija / *Chemistry* FMF – UN in VS
Osnove kemije / *Fundamentals of Chemistry* FGG – UN
Splošna kemija / *General Chemistry* BF – UN
Anorganska kemija / *Inorganic Chemistry* FFA – UN
Splošna in organska kemija / *General and* Organic *Chemistry* FFA – UN
Anorganska kemija / *Inorganic Chemistry* NTF – UN
Splošna in fizikalna kemija / *General and Physical Chemistry* BF – UN (1. st)
Anorganska kemija / *Inorganic Chemistry* PEF – UN
Bioanorganska kemija / *Bioinorganic Chemistry* BF – UN
Strukturna kemija / *Structural Chemistry* PEF – UN

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 Applications in Catalysis*

- Študij interakcij kovinskih ionov z biološko aktivnimi ligandi kinoloni in protiviralnimi nukleotidnimi analogi / *Studies of Interactions of Metal Ions with Biologically Active Quinolone Ligands and Anti-Viral Nucleotide Analogues*
- Rentgenska strukturna analiza monokristalov (koordinacijske in organske spojine) ter prahov (keramika) / *X-Ray Structure Analysis of Single Crystals (Coordination and Organic Compounds) and Powders (Ceramics)*
- Sol-gel priprava organsko-anorganskih hibridov z ionsko prevodnostjo / *Sol-Gel Preparation of Organic-Inorganic Hybrids Exhibiting Ionic Conductivity*
- Koordinacijske spojine platine, ki so potencialno uporabne kot citostatiki in virostatiki / *Coordination Compounds of Platinum, Potentially Applicable as Cytostatics and Virostatics*
- Vezava kovinskih ionov na biološke makromolekule, kot je npr. hialuronska kislina / *Bonding of Metal Ions on Bilogical Macromolecules such as Hialuronic Acid*
- Imobilizacija kovinskih zvrsti v kontaminirani zemlji / *Immobilization of Metal Species in Contaminated Soil*
- Imobilizacija kovinskih zvrsti v onesnaženih tleh in trdnih odpadkih / *Immobilization of Metal Species in Contaminated Soil and Solid Waste*
- 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

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- P. Šegedin, Priznanje najboljšega predavatelja na študijskem programu Kemija v študijskem letu 2007/2008 po izboru študentov / *Students Award as the Best Lecturer on Chemistry Study Programme in the School Year 2007/2008*

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

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

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL SCIENTIFIC CONFERENCES

- I. Leban, sopredsednik organizacijskega odbora 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«, eksperimentalno predavanje za popularizacijo kemije / *"Researcher's Night" – Demonstration Lecture for the Popularization of Chemistry*
- S. Petriček, predsednica Državne predmetne komisije za splošno maturo iz kemije / *President of the Subject Testing Committee for the Matura in Chemistry*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Modularni sistem za termično analizo – Mettler Toledo (TGA/SDTA 851, DSC 822, HP DSC 827) / *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*
- Planetarni mlin PM100 Retsch / *Planetar Mill PM100 Retsch*

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.: Ekspertne storitve (letna pogodba) / *Expert Services (Annual Contract)*
- Salonit d.d.: Kvantitativne fazne analize (letna pogodba) / *Quantitative Phase Analyses (Annual Contract)*

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

ESS (Evropski socialni sklad –projekti / *European Social Fund*
Partnerstvo fakultet in šol: vseživljenjsko učenje učiteljev naravoslovnih predmetov / *Partnership of 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
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 Aluminium-Titanium(IV) Phosphates, Phosphonates, Phosphinates and Fluorides* Nosilec / *Principal Researcher*: A. Demšar
Slovenija – Srbija *Slovenia – Serbia*	Struktura in mikrostruktura oksidnih nanomaterialov / *Structure and Microstructure of Oxide Nanomaterials* Nosilec / *Principal Researcher*: A. Meden
Slovenija – Avstrija *Slovenia – Austria*	Rutenijeve spojine in njihova možna uporaba v elektrokemoterapiji / *Ruthenium Compounds and their Possible Applications in Electrochemotherapy* Nosilec / *Principal Researcher*: I. Turel

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

Prof. Dr. Aleksandar Kremenović, University of Belgrade, Faculty of Mining and Geology, and Dr. Bratislav Antić, The Vinča Institute of Nuclear Sciences, Belgrade, Serbia, *XRPD Line Broadening Analysis and Microstructure Parameters in Oxide Nanomaterials; Magnetic Nanoparticles: Relationship between Crystal Structure (Microstructure) and Magnetism,* December 2008

BIBLIOGRAFIJA 2008 / REFERENCES 2008

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

AK1. PADEŽNIK GOMILŠEK, Jana, CERC KOROŠEC, Romana, BUKOVEC, Peter, KODRE, Alojz. EXAFS and IR analysis of electrochromic NiO[sub]x/NiO[sub]xH[sub]y thin films. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 1, str. 154–159. [COBISS.SI-ID 29362693]

AK2. SIMONIČ, Igor, ZUPANČIČ, Silvo, GOLOBIČ, Amalija, GOLIČ, Ljubo, STANOVNIK, Branko. The crystal structure of lacidipine phototransformation product. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 2, str. 458–461. [COBISS.SI-ID 29570053]

AK3. DOLENC, Darko, MODEC, Barbara. Alkylation of amines with alcohols and carboxylate esters : the origin of N-methylpyridinium cations in the synthesis of pyridine-molybdate(V) complexes. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 4, str. 752–756. [COBISS.SI-ID 30080261]

AK4. KITANOVSKI, Nives, GOLOBIČ, Amalija, ČEH, Boris. Synthesis and characterization of Mo(V)-oxido complexes containing the thiocyanato-N ligand. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 4, str. 767–774. [COBISS.SI-ID 30080517]

AK5. DOJER, Brina, KRISTL, Matjaž, JAGLIČIĆ, Zvonko, DROFENIK, Mihael, MEDEN, Anton. Ammoniumbis (hydroxylammonium) pentafluoridooxidovanadate(IV) : synthesis and characterisation of a new fluorovanadate. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 4, str. 834–840. [COBISS.SI-ID 30084101]

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izr. prof. dr. Metka Renko

v dopolnilnem razmerju:
prof. dr. Tamara Lah Turnšek
prof. dr.Vladka Čurin Šerbec
izr. prof. dr. Kristina Djinović Carugo
izr. prof. dr. Roman Jerala
izr. prof. dr. Boris Turk
izr. prof. dr. Janez Plavec

Asistenti / Assistants
doc. dr. Marko Dolinar
dr. Petra Prijatelj Žnidaršič
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* – UN
- Biokemijska informatika / *Bioinformatics* – UN
- Encimatika / *Enzymology* – UN
- Tehnologija rekombinantne DNA / *Recombinant DNA Technology* – UN
- Molekularna imunologija / *Molecular Immunology* – UN
- Metode določanja 3D strukture makromolekul / *Methods of 3D Structure Determination of Macromolecules* – UN
- Encimska tehnologija / *Enzyme Technology* – UN
- Biološke membrane / *Biological Membranes* – UN
- Kemija in biokemija živil / *Chemistry and Biochemistry of Food* – UN
- Regulacija metabolizma / *Regulation of Metabolism* – UN
- Biokemija raka / *Biochemistry of Cancer* – UN
- Encimi / *Enzymes* – UN
- Biokemija II / *Biochemistry II* – UN

Podiplomski programi / *Postgraduate Programmes*

- Biološke makromolekule / *Biological Macromolecules*

IZVEN FKKT / EXTRAMURAL COURSES

Dodiplomski programi / *Undergraduate Programmes*

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

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

- Izbrani procesi iz biokemije in molekularne biologije / *Selected Topics in Biochemistry and Molecular Biology*
- Načela in tehnike v biokemiji in molekularni biologiji / *Principles and Methods in Biochemistry and Molecular Biology*
- Genetika / *Genetics*
- Jedrska magnetna resonanca za raziskave bioloških makromolekul / *Nuclear Magnetic Resonance for Investigations of Biological Macromolecules*
- Molekularna bioinformatika / *Molecular Bioinformatics*
- Eksperimentalne metode v raziskavah naravne imunosti / *Experimental Methods in Natural Immunity Research*

Monoklonska protitelesa – pregled področja in možnosti njihove uporabe v raziskavah, diagnostiki in terapiji / *Monoclonal Antibodies – Review and Their Application for Research, Diagnostics and Therapy.*

Metode v eksperimentalni onkologiji / *Methods in Experimental Oncology*

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 specifične vezavne proteine.

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

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

Cianobakterije so bogat vir biološko aktivnih metabolitov. Med njimi sta dve skupini cikličnih peptidov, ki sta poznani kot inhibitorji serinskih peptidaz, in sicer depsipeptidi ter peptidi, ki vsebujejo ureido vez. V okviru tega projekta (nosilka prof.dr. Tamara Lah) smo okarakterizirali tri takšne spojine, planktopeptin BL1125 ter anabenopeptidna B in F. Naša naloga je bila določiti selektivnost peptidov za različne peptidaze, identificirati mehanizem inhibicije ter določiti kinetične parametre interakcij. Naši eksperimenti so pokazali, da je planktopeptidin BL1125 močan inhibitor levkocitne in pankreasne elastaze ter kimotripsina, medtem ko anabenopeptina inhibirata le obe elastazi.

Na osnovi sinteznobiološkega klonirnega vektorja pSB1 smo pripravili ekspresijski vektor pMD204 z modularno zgradbo, ki omogoča enostavno pripravo fuzijskih proteinov, hkrati pa s preprostim posegom na ravni DNA lahko določimo lokalizacijo rekombinantnega proteina, ne da bi bilo treba zamenjati vektor. Novi ekspresijski vektor omogoča zamenjavo regulatornih regij s kasetno mutagenezo, njegovo delovanje pa smo preizkusili na primeru inhibitorja cisteinskih proteinaz, kokošjega cistatina, ki smo ga pripravili v aktivni obliki v periplazmi ali citoplazmi bakterij *Escherichia coli*.

V letu 2008 smo se začeli ukvarjati z raziskavami človeške transmembranske celične adhezijske molekule EpCAM in sorodnega proteina Trop2 s strukturnega (določitev kristalne strukture) in funkcijskega vidika (interakcije z α-aktininom in drugimi znotrajceličnimi ter zunajceličnmi proteini). Raziskava je relevantna tudi z medicinskega vidika, saj se EpCAM prekomerno ali

»*de novo*« izraža na številnih tumorjih epitelnega izvora in kot tak predstavlja zanimivo tarčo bodočih antitumorskih terapij. V okviru teh študij in drugih študij smo tudi osnovno opremili laboratorij za delo s kulturami insektnih celic za pripravo rekombinantnih proteinov v večjih količinah ter s kulturami celic višjih sesalcev.

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

The 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 specific binding proteins.

Co-workers 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. We exchanged potentially immunogenic sites on the surface of the murine immunoglobulin with human counterparts. As next, we expressed single-chain antibody fragments of the murine and humanized antibodies in bacterial cells.

Cyanobacteria are a rich source of biologically active metabolites. Two groups of cyclic peptides, depsipeptides and ureido linkage-containing peptides were previously reported to inhibit serine peptidases. In this project (project leader Prof. Tamara Lah Turnšek) we have characterized three such substances, planktopeptin BL1125 and anabaenopeptins B and F. Our task was to determine the selectivity of the peptides towards different peptidases, to identify the mechanism of inhibition and to calculate the kinetic parameters. The results of our experiments have shown that planktopeptin BL1125 is a tight-binding inhibitor of leukocyte and pancreatic elastases as well as chymotrypsin, while the anabeanopeptins inhibited both elastases.

On the basis of the synthetic biology cloning vector pSB1 we prepared a modullary assembled expression vector (named pMD204) which allows for an easy preparation of fusion proteins. A simple manipulation of the vector can change the localization of the recombinant protein. In addition, regulatory regions can be exchanged by cassette mutagenesis. We proved the versatility and usefulness of the vector with chicken cystatin, a cysteine proteinase inhibitor, which we obtained in an active form either in the periplasm or in the cytoplasm of Escherichia coli.

In the year 2008 we started research on human transmembrane cell adhesion molecule EpCAM and on the related protein Trop2 from structural (determination of crystal structure) and functional aspect (interactions with α-actinin and other intra- and extracellular proteins). The research is also relevant from the medical perspective since EpCAM in overexpressed or even "de novo" expressed on various tumors of epithelial origin and is as such an interesting target of future antitumor therapies. In the light of this and other studies we also established laboratory with basic equipment for working with insect cell cultures (preparation of recombinant protreins in larger quantities) and cultures of cells of higher mammals.

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- Marca 2008 je M. Dolinar prejel Sokratovo odličje za visokošolsko didaktiko »Sova«, ki ga podeljuje Slovensko društvo za visokošolsko didaktiko. Priznanje je dobil »za posebej zavzeto in odlično pedagoško delo, za širjenje novih in uspešnih učnih metod ter za zasluge pri razvoju slovenske visokošolske didaktike« / *In March 2008, M. Dolinar was awarded Socrates Prize for Higher Education Didactics for his »outstanding and excellent pedagogic work, broadening of new and successful teaching methods and for his credits for development of Slovenian higher education didactics«.*
- Univerzitetno študentsko Prešernovo nagrado za leto 2008 je dobila Nina Erčulj, študentka biokemije, za svoje raziskovalno delo s področja tehnologije rekombinantne DNA, ki ga je opravila na naši katedri pod mentorstvom M. Dolinarja / *Biochemistry student Nina Erčulj was recipient of the 2008 University Prešeren Award for her research in the field of recombinant DNA technology performed at our Chair under the mentorship of M. Dolinar.*
- J. Plavec je dobil priznanje najboljšega predavatelja na študijskem programu Biokemija v študijskem letu 2007/2008 po izboru študentov / *Students Award as the Best Lecturer on Biochemistry Study Programme in the School Year 2007/2008.*

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)

RAZISKOVALNI PROJEKTI / RESEARCH PROJECTS

L3–0206	Prioni v humani medicini: od strukturnih študij do aplikacij / *Prions in Human Medicine: From Structural Studies to Applications* Nosilka / *Principal Researcher*: V. Čurin Šerbec
J1–0841	Antikancerogeno delovanje bioaktivnih spojin cianobakterijskega izvora v napredovanju možganskih tumorjev –gliobastomov / *Anticarcinogenic Activity of Bioactive Compounds from Cyanobacterial Source in the Progression of Brain Tumours – Glioblastoma* Nosilka / *Principal Researcher*: T. Lah Turnšek

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KATEDRA ZA FIZIKALNO KEMIJO
CHAIR OF PHYSICAL CHEMISTRY

PREDSTOJNIK KATEDRE / HEAD

prof. dr. Jože Koller

SODELAVCI KATEDRE / PERSONNEL

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prof. dr. Marija Bešter Rogač
izred. prof. dr. Andrej Jamnik
izred. prof. dr. Ksenija Kogej
prof. dr. Jože Koller
izred. prof. dr. Jurij Lah
prof. dr. Ciril Pohar
prof. dr. Jože Škerjanc, zaslužni profesor (upokojen) / *Professor Emeritus*
prof. dr. Gorazd Vesnaver
prof. dr. Vojeslav Vlachy

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

Raziskovalci / Researchers
dr. Jožica Dolenc
dr. Irena Lipar

Strokovni sodelavec / Research Assistant
Aleksander Vrhovšek, univ. dipl. ing. kem.

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

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 – UN in VS
Fizikalna kemija / *Physical Chemistry* NTF – UN
Fizikalna kemija / *Physical Chemistry* PEF – UN
Fizikalna kemija II / *Physical Chemistry II* PEF – UN
Procesna tehnika v živilstvu II / *Process Techniques in Food Technology II* BF – UN
Vaje iz fizikalne kemije / *Physical Chemistry Laboratory* FMF – UN

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 Properties of Different Stereoregular Polyelectrolytes* Termodinamične in transportne lastnosti raztopin ionenov z različnimi protiioni / *Transport Properties of Ionene Solutions with Different Counter Ions*
– Raziskave soli polianetolesulfonske kisline / *Studies of Polyanetholesulfonic Acid and its Alkaline Salts*
– Interakcije med površinsko aktivnimi snovmi in polielektroliti / *Interactions Among Surface Active Compounds and Polyelectrolytes*

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

– U. Bren, Nagrada Maksa Samca za najboljši doktorat (mentor J. Mavri, somentor J. Koller) / *The Maks Samec Award for the Best PhD Thesis*

– T. Sajevic, Prešernova nagrada FKKT za leto 2008 (mentor J. Reščič) / *The Faculty Prešeren Award for 2008*

– A. Korenčič, Prešernova nagrada FKKT za leto 2008 (mentor J. Lah) / *The Faculty Prešeren Award for 2008*

– A. Godec et al., Priznanje Slovenske znanstvene fundacije: Prometej znanosti za odličnost v komuniciranju za leto 2008 / *SZF Award: Prometheus in Science for Excellence in Communication for 2008*

– V. Vlachy, izvolitev za rednega člana Evropske akademije znanosti in umetnosti / *Elected to the European Academy of Sciences and Arts (Academia Scientiarum et Artium Europaea)*

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

M. Bešter Rogač, članica uredniškega odbora / *Editorial Board Member*, *J. Mol. Liq.* 2008– Amsterdam, Elsevier.

M. Bešter Rogač, članica uredniškega odbora / *Editorial Board Member, Acta Chimica Slovenica, 2004–*

G. Vesnaver, član uredniškega odbora / *Editorial Board Member*, *Acta Chimica Slovenica*, 1998–

DRUGO / OTHER

- M. Bončina, Ad Futura polletna štipendija za doktorski študij 2008 / *Six – Month Ad Futura Fellowship for Doctoral Study*
- J. Dolenc, podoktorska štipendija na Zvezni tehniški visoki šoli (ETH), Zürich / *Post Doctoral Fellowship at ETH*, *Zürich*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Diferenčni dinamični kalorimeter N-DSC II (CSC, ZDA) */ Nano II Differential Scanning Calorimeter II (CSC, USA)*
- UV-VIS Spektrophotometer Cary BIO 100 (Varian, Avstralija)
- CD Spectrometer 62A DS (Aviv, ZDA)
- Titracijski mikrokalorimeter VP-ITC (Microcal, ZDA) / *Isothermal Titration Microcalorimeter VP-ITC (Microcal, USA)*
- Računalniška gruča iz 12 dvoprocesorskih računalnikov AMD MP 2600+ */ 12-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-Core AMD Athlon 64 X2 4200+ Server CPUs*
- Računalniška gruča iz 8 štirijedrnih 64 bitnih Intel Q9550 procesorjev / *Eight- Node Computer Cluster Based on Quad-Core Intel Q9550 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, Ther-*

mostat 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*
– TV100K termostatirana dvojna enota za gelsko elektroforezo ter Syngen G:BOX temnica s kamero /*TV100K Cooled Twin-Plate Mini-Gel Electrophoresis Unit & Syngen G:BOX Darkroom with Camera*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

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

TEMELJNI PROJEKTI / BASIC RESEARCH

Z1–9576 Simulacije molekulske dinamike nukleinskih kislin: struktura, dinamika in termodinamska stabilnost / *Molecular Dynamics Simulations of Nucleic Acids*: *Structure, Dynamics and Thermodynamic Stability*
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.

Pogodba št. I/8-106259/2008 Študij in analiza farmacevtskih materialov / *Studies and Analysis of Pharmaceutical Materials*
Nosilec / *Principal Researcher*: J. Koller
Financer / *Sponsored by*: Krka d.d.

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

– A. Godec, mentor slovenske srednješolske ekipe na mednarodni kemijski olimpijadi v Budimpešti 2008 / *Mentor of the Slovenian Team at the International Chemistry Olympiad, Budapest, 2008*

– 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 Gunsteren),* 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 – Madžarska *Slovenia – Hungary*	Obravnava strukture kompleksnih tekočin z metodama ozkokotnega rentgenskega sipanja in reverzne simulacije Monte Carlo / *Understanding the Structure of Complex Liquids by Small Angle Scattering and Reverse Monte Carlo Simulation* Nosilec / *Principal Researcher*: A. Jamnik
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)
Slovenija – Portugalska *Slovenia – Portugal*	Vpliv hidrofobnosti in togosti polimerne verige na interakcije med polielektroliti in surfaktanti/ *Effect of the Polymer Hydrophobicity and Backbone Rigidity on Polyelectrolyte-Surfactant Interactions* Nosilec / *Principal Researcher*: Ksenija Kogej

DRUGE OBLIKE MEDNARODNEGA SODELOVANJA / OTHER FORMS OF INTERNATIONAL COOPERATION

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

– V. Vlachy, *Polyelectrolyte Hydratation: New Experiments, Theory, and Simulations,* University of Puerto Rico, Department of Physics, San Juan, Puerto Rico,USA, February 2008
– V. Vlachy, *Can Polyelectrolyte Studies Help to Understand Hydration of Biologically Important Solutes*, University of California at San Francisco, San Francisco, USA, May 2008

- M. Bončina, *Solvent-Mediated Interactions Between Dipeptides in Aqueous Urea Solution,* Max Planck Institute for Polymer Research, Mainz, Germany, June 2008
- I. Prislan, J. Lah, Č. Podlipnik, *Thermodynamics of Multivalent Ligand Binding to Cholera Toxin,* Utrecht University, The Netherlands, December 2008
- J. Reščič, *Depletion Interaction and Salt- Specific Effects in Protein Solutions,* Department of Chemistry, University of Coimbra, Portugal, November 2008
- Č. Podlipnik, *Molecular Design of Cholera Toxin Inhibitors,* Università degli Studi di Milano, Milano, Italy, June 2008
- J. Dolenc, *How to Analyse Using GROMOS Biomolecular Modelling Retreat*, The University of Queensland, Brisbane, Australia, September 2008
- J. Dolenc, *Hydration of a Trimeric Alpha-Helical Coiled Coil*, Paul Scherrer Institute (PSI), Villigen, Switzerland, April 2008
- T. Urbič, *Phase Diagrams: Analytical Modelling*, University of California at San Francisco, San Francisco, USA, October 2008

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

- Dr. Per Hansson, University of Uppsala, Sweden, *A Theory of Surfactant Self-Assembly in Oppositely Charged Polymer Networks,* January 2008
- Prof. Dr. Remy Loris, Instituut voor Moleculaire Biologie, Vrije Universiteit Brussel and Vlaams Instituut voor Biotechnologie, *Unraveling the Molecular Mechanisms in the CCD Addiction Machinery,* March 2008
- Dr. Beatriz Millan Malo, Departamento de Nanotecnologija, Centro de Fisica Aplicada y Tecnologia Avanzada, Universidad Nacional Autonoma de Mexico, Mexico, *Application of SAFT-VR in the Design of Chemical Process,* September 2008
- Dr. Sebastian Rast, Max-Planck Institut für Meteorologie, Hamburg, Germany, *Chemistry and Aerosols in the Atmosphere – Recent Results of the Global Simulation Programs ECHAM5-MOZ (RETRO) and ECHAM5-HAMMOZ (TRACE-P),* September 2008
- Dr. Rita Dias, University of Coimbra, Portugal, *Experiments and Simulations on Colloidal Systems. DNA Compaction,* September 2008
- Dr. Jens Norrman, University of Lund, Sweden, *Controlling Structure and Water Uptake of Polyion – Surfactant Ion Complex Salts*, October 2008

BIBLIOGRAFIJA 2008 / REFERENCES 2008

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

FK1. BEŠTER-ROGAČ, Marija. Determination of the limiting conductances and the ion-association constants of calcium and manganese sulfates in water from electrical conductivity measurements. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 1, str. 201–208. [COBISS.SI-ID 29362181]

FK2. URBIČ, Tjaša, URBIČ, Tomaž, AVBELJ, Franc, DILL, Ken A. Molecular simulations find stable structures in fragments of protein G. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 2, str. 385–395. [COBISS.SI-ID 29569797]

FK3. PIÑERO, Jesus, BHUIYAN, Lutful B., REŠČIČ, Jurij, VLACHY, Vojko. Thermodynamics and structural properties of the model polyelectrolyte-electrolyte mixture. *Acta chim. slov.*. [Tiskana izd.], 2008, letn. 55, št. 3, str. 521–527, graf. prikazi. [COBISS.SI-ID 29801477]

FK4. VLACHY, Vojko. The distribution of ions between a bulk electrolyte solution and charged microcapillaries in solvents with low dielectric constant. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 4, str. 815–821. [COBISS.SI-ID 30080773]

FK5. KOGEJ, Ksenija. Binding of cationic surfactants by kappa, iota and lambda carrageenans in aqueous solution in the presence of sodium chloride. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 4, str. 985–991. [COBISS. SI-ID 30082309]

FK6. CERAR, Janez, PODLIPNIK, Črtomir. Relationships between aqueous acidities of benzene polycarboxylic acids and computed surface-electrostatic potential and charges. *Acta chim. slov.*. [Tiskana izd.], 2008, vol. 55, no. 4, str. 999–1008. [COBISS.SI-ID 30083333]

FK7. BONČINA, Matjaž, REŠČIČ, Jurij, VLACHY, Vojko. Solubility of lysozyme in polyethylene glycol-electrolyte mixtures : the depletion interactions and ion-specific effects. *Biophys. j.*, 2008, vol. 95, no. 3, str. 1285–1294. [COBISS.SI-ID 29681413]

FK8. DOLENC, Jožica, BARON, Riccardo, MISSIMER, John, STEINMETZ, Michael O., GUNSTEREN, Wilfred F. van. Exploring the conserved water site and hydratation of a coiled-coil trimerisation motif : a MD simulation study. *ChemBioChem*. [Print ed.], 2008, vol. 9, no. 11, str. 1749–1756. [COBISS.SI-ID 30052613]

FK9. DRUCHOK, M., HRIBAR, Barbara, KRIENKE, H., VLACHY, Vojko. A molecular dynamics study of short-chain polyelectrolytes in explicit water : toward the origin of ion-specific effects. *Chem. Phys. Lett.*. [Print ed.], 2008, vol. 450, no. 4/6, str. 281–285. [COBISS.SI-ID 29167109]

FK10. SIMONČIČ, Zvone, ROŠKAR, Robert, GARTNER, Andrej, KOGEJ, Ksenija, KMETEC, Vojko. The use of micro-calorimetry and HPLC for the determination of degradation kinetics and thermodynamic parameters of Perindopril Erbumine in aqueous solutions. *Int. j. pharm.*. [Print ed.], 2008, no. 1–2, vol. 356, str. 200–205. [COBISS.SI-ID 2273393]

FK11. BEŠTER-ROGAČ, Marija. Electrical conductivity of concentrated aqueous solutions of divalent metal sulfates. *J. chem. eng. data*, 2008, vol. 53, no. 6, str. 1355–1359. [COBISS.SI-ID 29568005]

FK12. PIÑERO, Jesus, BHUIYAN, Lutful B., REŠČIČ, Jurij, VLACHY, Vojko. Ionic correlations in the inhomogeneous atmosphere surrounding cylindrical polyions : catalytic effects of polyions. *J. chem. phys.*, 2008, vol. 128, no. 21, art. no. 214904 (10 str.), graf. prikazi. [COBISS.SI-ID 29587717]

FK13. JAMNIK, Andrej. Simulating asymmetric colloidal mixture with adhesive hard sphere model. *J. chem. phys.*, 2008, vol. 128, no. 23, art. no. 234504 (10 str.), graf. prikazi. [COBISS.SI-ID 29744133]

FK14. REŠČIČ, Jurij, LINSE, Per. Potential of mean force between charged colloids : effect of dielectric discontinuities. *J. chem. phys.*, 2008, vol. 129, no. 11, art. no. 114505 (9 str.), graf. prikazi. [COBISS.SI-ID 29795333]

FK15. TOMŠIČ, Matija, PROSSNIGG, Florian, GLATTER, Otto. A thermoreversible double gel : characterization of a methylcellulose and [kappa]-carrageenan mixed system in water by SAXS, DSC and rheology. *J. colloid interface sci.*, 2008, vol. 322, no. 1, str. 41–50. [COBISS.SI-ID 29506309]

FK16. ZEGA, Anamarija, SRČIČ, Stanko, MAVRI, Janez, BEŠTER-ROGAČ, Marija. Molecular interactions of 1,4-dihydropyridine derivatives with selected organic solvents : a volumetric, spectroscopic and computational study. *J. mol. struct.*. [Print ed.], 2008, issues 1/3, vol. 875, str. 354–363. [COBISS.SI-ID 3741978]

FK17. KOVAČIČ, Saša, KOLLER, Jože, CERKOVNIK, Janez, TUTTLE, Tell, PLESNIČAR, Božo. Dihydrogen trioxide clusters, (HOOOH)[sub]n (n = 2-4), and the hydrogen-bonded complexes of HOOOH with acetone and dimethyl ether : implications for the decomposition of HOOOH. *J. phys. chem., A Mol. spectrosc. kinet. environ. gen. theory*, 2008, vol. 112, no. 35, str. 8129–8135, graf. prikazi. [COBISS.SI-ID 29912837]

FK18. CERAR, Janez, ŠKERJANC, Jože. Electric transport and ion binding in solutions of fullerenehexamalonic acid T[sub]h-C[sub](66)(COOH)[sub](12) and its alkali and calcium salts. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2008, vol. 112, no. 3, str. 892–895. [COBISS.SI-ID 29207045]

FK19. MAY, Sylvio, IGLIČ, Aleš, REŠČIČ, Jurij, MASET, Stefano, BOHINC, Klemen. Bridging like-charged macroions through long divalent rodlike ions. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2008, vol. 112, no. 6, str. 1685–1692. [COBISS.SI-ID 29259525]

FK20. CERAR, Janez, URBIČ, Tomaž. Viscosity and electrophoretic mobility of cesium fullerenehexamalonate in aqueous solutions : comparing experiments and theories on nanometer-sized spherical polyelectrolyte. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2008, vol. 112, no. 39, str. 12240–12248. [COBISS.SI-ID 29871621]

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FK23. BONČINA, Matjaž, APELBLAT, Alexander, BARTHEL, Josef, BEŠTER-ROGAČ, Marija. Investigation of the dissociation and dimerization of cyclamic acid in aqueous solutions by means of a conductometric method. *J. solution chem.*, 2008, vol. 37, no. 11, str. 1561–1574. [COBISS.SI-ID 29794821]

FK24. PRISLAN, Iztok, LAH, Jurij, VESNAVER, Gorazd. Diverse polymorphism of G-quadruplexes as a kinetic phenomenon. *J. Am. Chem. Soc.*, 2008, vol. 130, no. 43, str. 14161–14169, graf. prikazi. [COBISS.SI-ID 29937669]

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FK27. JARDAT, Marie, HRIBAR, Barbara, VLACHY, Vojko. Self-diffusion coefficients of ions in the presence of charged obstacles. *PCCP. Phys. chem. chem. phys. (Print)*, 2008, vol. 10, no. 3, str. 449–457. [COBISS.SI-ID 29166853]

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FK29. ZHOU, Shiqi, JAMNIK, Andrej. Structural properties of a model system with effective interparticle interaction potential applicable in modeling of complex fluids. *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, 2008, vol. 112, no. 44, str. 13862–13872. [COBISS.SI-ID 30109445]

PREGLEDNI ZNANSTVENI ČLANEK / REVIEW ARTICLE

FK30. GUNSTEREN, Wilfred F. van, DOLENC, Jožica. Biomolecular simulation : historical picture and future perspectives. *Biochem Soc Trans*, 2008, vol. 36, no. 1, str. 11–15. [COBISS.SI-ID 29229829]

FK31. GUNSTEREN, Wilfred F. van, DOLENC, Jožica, MARK, Alan E. Molecular simulation as an aid to experimentalists. *Curr. Opin. Struct. Biol.*. [Print ed.], 2008, vol. 18, no. 2, str. 149–153. [COBISS.SI-ID 29462021]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

FK32. PRISLAN, Iztok, LAH, Jurij, VESNAVER, Gorazd. Kinetika – še en košček sestavljanke razumevanja zvitja in razvitja d(G[spodaj]4T[spodaj]4G[spodaj]3)[spodaj]2 kvadrupleksa = Using kinetics to solve the puzzle of folding and unfolding of d(G[sub]4T[sub]4G[sub]3)[sub]2 quadruplex. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, [1–10] str., graf. prikazi. [COBISS.SI-ID 29848069]

FK33. LUKŠIČ, Miha, HRIBAR, Barbara, VLACHY, Vojko, BUCHNER, Richard. Vloga meddelčnih interakcij v vodnih raztopinah ionenov = The role of interparticle interactions in aqueous solutions of ionenes. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, [1–10] str., graf. prikazi. [COBISS.SI-ID 29847301]

FK34. URBIČ, Tomaž, VLACHY, Vojko. Preprosti statistično-mehanski model vode = A simple statistical mechanical model of water. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, [1–7] str., graf. prikazi. [COBISS.SI-ID 29847045]

FK35. CERAR, Janez, PODLIPNIK, Črtomir. Zveza med elektrostatskim potencialom na površini benzenovih polikarboksilnih kislin in njihovimi ionizacijskimi konstantami = Relationship between surface-electrostatic potential and ionization constants of benzene polycarboxylic acids. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, [1–8] str., graf. prikazi. [COBISS.SI-ID 29847557]

FK36. PODLIPNIK, Črtomir. Naravni polifenoli kot inhibitorji katalitsko aktivne enote A[spodaj]1 toksina kolere = Natural polyphenols as inhibitors of catalitically active A[sub]1 cholere toxin unit. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). *Slovenski kemijski dnevi 2008, Maribor, 25. in 26. september 2008 : [zbornik referatov]*. Maribor: Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo, 2008, str. [1–10], graf. prikazi. [COBISS.SI-ID 29841925]

FK37. HAUPTMAN, Nina, KLANJŠEK GUNDE, Marta, MAČEK, Marijan, BEŠTER-ROGAČ, Marija. Electrical properties of epoxy-based carbon black nanocomposite and its technological reliability. V: *XX kongres na hemičarite i tehnolozite na Makedonija : izvodi od soopštenijata : abstract book*. Skopje: Sojuz na hemičarite i tehnolozite na Makedonija, 2008, str. 1–4. [COBISS.SI-ID 4012314]

FK38. PRISLAN, Iztok, PODLIPNIK, Črtomir, GAMS, Matjaž. Genetski algoritem in metoda Monte Carlo v programu AutoDock. V: BOHANEC, Marko (ur.), GAMS, Matjaž (ur.), RAJKOVIČ, Vladislav (ur.), URBANČIČ, Tanja (ur.), BERNIK, Mojca (ur.), MLADENIĆ, Dunja (ur.), GROBELNIK, Marko (ur.), HERIČKO, Marjan (ur.), KORDEŠ, Urban (ur.), MARKIČ, Olga (ur.). *Zbornik 11. mednarodne multikonference Informacijska družba – IS 2008, 13.–17. oktober 2008 : zvezek A : volume A*, (Informacijska družba). Ljubljana: Institut »Jožef Stefan«, 2008, str. 85–88. [COBISS.SI-ID 22105383]

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

FK39. GAŠPERLIN, Mirjana, BEŠTER-ROGAČ, Marija, Physicochemical Characterization of Pharmaceutically Applicable Microemulsions: Tween 40/Imwitor 308/Isopropyl Myristate/Water. V Monzer Fanun (Ed.) *Microemulsions: Properties and Applications*, Chapter 10, CRC Press, Taylor & Franciss Group, 2008.

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

FK40. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta, KOS, Zvonka (ur.), FORTUNA, Špela (ur.). *Il mio primo approccio alla chimica 1 : chimica per la classe VIII della scuola elementare, Quaderno attivo*. 1a ed. Lubiana: Modrijan, 2008. 116 str., ilustr. ISBN 978-961-241-193-0. [COBISS.SI-ID 236835328]

FK41. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Il mio primo approccio alla chimica 2 : chimica per la classe IX della scuola elementare*. 2a ed. Ljubljana: Modrijan, 2008. 112 str., ilustr. ISBN 978-961-241-123-7. [COBISS.SI-ID 239361024]

FK42. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta, FORTUNA, Špela (ur.). *Il mio primo approccio alla chimica 2 : chimica per la classe IX della scuola elementare, Quaderno attivo*. 1a ed. Lubiana: Modrijan, 2008. 96 str., ilustr. ISBN 978-961-241-236-4. [COBISS.SI-ID 238271232]

FK43. GLAŽAR, Saša A., GODEC, Andrej, VRTAČNIK, Margareta, WISSIAK GRM, Katarina Senta. *Moja prva kemija 1 : kemija za 8. razred osnovne šole, Delovni zvezek*. 5. izd. Ljubljana: Modrijan, 2008. 116 str., ilustr. ISBN 978-961-6465-82-3. [COBISS.SI-ID 238096896]

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PREDAVANJE NA TUJI UNIVERZI / INVITED LECTURE AT FOREIGN UNIVERSITY

FK46. DOLENC, Jožica. *How to analyse using GROMOS : vabljeno predavanje : [Biomolecular modeling retreat 2008, September 2008, The University of Queensland, Australia]*. Brisbane, 2008. [COBISS.SI-ID 30053637]

FK47. DOLENC, Jožica. *Hydration of a trimeric alpha-helical coiled coil : vabljeno predavanje : [Paul Scherrer Institute (PSI), Laboratory of Physical Chemistry, ETH Zurich, April 29, 2008]*. Zurich, 2008. [COBISS.SI-ID 29462277]

FK48. PODLIPNIK, Črtomir. *Molecular design of cholera toxin inhibitors : [Università degli Studi di Milano, Via Venezian Milano, 4. 6. 2008]*. 2008; Milano. [COBISS.SI-ID 29555461]

FK49. URBIČ, Tomaž. *Phase diagrams: analytical modeling : [Department of Pharmaceutical Chemistry and Graduate Group in Biophysics, University of California, San Francisco, USA, 1. 10. 2008]*. San Francisco, 2008. [COBISS.SI-ID 29872389]

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FK51. BONČINA, Matjaž. *Solvent-mediated interactions between dipeptides in aqueous urea solution : [Max Planck Institute for Polymer Research, Mainz, Germany, 4. 6. 2008]*. Mainz, 2008. [COBISS.SI-ID 29575429]

FK52. REŠČIČ, Jurij. *Depletion interaction and salt-specific effects in protein solutions : [Department of Chemistry, University of Coimbra, Portugal, 28. 11. 2008]*. Coimbra, 2008. [COBISS.SI-ID 30193925]

FK53. VLACHY, Vojko. *Can polyelectrolyte studies help to understand hydration of biologically important solutes : [University of California, San Francisco, 23. 5. 2008]*. San Francisco, 2008. [COBISS.SI-ID 30194181]

FK54. VLACHY, Vojko. O *vplivu hidrofobnih skupin na interakcijo med dvema nabojema v raztopini : Seminar Društva biofizikov Slovenije, Institut Jožef Stefan, Ljubljana, 18. november 2008*. Ljubljana, 2008. [COBISS.SI-ID 30194437]

UREDNIK / EDITOR

FK55. *Acta chimica slovenica*. Vesnaver, Gorazd (član uredniškega odbora 1998–), Bešter-Rogač, Marija (član uredniškega odbora 2006–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. http://acta.chem-soc.si/. [COBISS.SI-ID 14086149]

FK56. *Journal of molecular liquids*. Bešter-Rogač, Marija (član uredniškega odbora 2008–). [Print ed.]. Amsterdam: Elsevier. ISSN 0167-7322. [COBISS.SI-ID 15382277]

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dr. Krištof Kranjc
Nenad Maraš, univ. dipl. kem.
dr. Jernej Wagger

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Tončka Kozamernik
Branka Miklavčič
Irena Povalej
Zdenka Sakelšek
Tatjana Stipanović

Mladi raziskovalci *Young researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Igor Pravst	M. Zupan	2003–2008	doktorski študij / *PhD*
Ana Bergant	J. Cerkovnik	2004–2009	doktorski študij / *PhD*
Vita Majce	S. Polanc	2007–2012	doktorski študij / *PhD*
Bojan Burja	S. Polanc	2005–2010	doktorski študij / *PhD*
Jure Hren	M. Kočevar	2006–2011	doktorski študij / *PhD*
Amadej Juranovič	M. Kočevar	2008–2012	doktorski študij / *PhD*
Črt Malavašič	J. Svete	2007–2011	doktorski študij / *PhD*
Lidija Pezdirc	J. Svete	2005–2008	doktorski študij / *PhD*
Gaj Stavber	M. Zupan	2005–2009	doktorski študij / *PhD*
Jernej Baškovč	B. Stanovnik	2007–2012	doktorski študij / *PhD*
Uroš Uršič	B. Stanovnik	2004–2009	doktorski študij / *PhD*

Ostali podiplomski študenti, ki niso v rednem delovnem razmerju / *Other postgraduate students*
Sanja Čavar
Žiga Nose

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*
Organska kemija / *Organic Chemistry* – UN – kemija / *Chemistry*
Organska kemija II / *Organic Chemistry II* – UN – kemija / *Chemistry*

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

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

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

Organska kemija / *Organic Chemistry* – VS

Organska analiza / *Organic Analysis* – UN

Splošna kemija II / *General Chemistry II* – VS

Spektroskopske metode / *Spectroscopic Methods* – UN

Analitika in spektroskopija / *Analysis and Spectroscopy* – VS

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

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

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

Organska kemija biološko pomembnih spojin / *Organic Chemisty of Biologically Importnat Compounds* – UN

Bioorganska kemija / *Bioorganic Chemistry* – UN

Usmerjena organska sinteza / *Directed Organic Synthesis* – UN

Bioaktivne spojine / *Bioactive Compounds* – UN

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

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

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

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

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 – UN

Kemija II / *Chemistry II* NTF – VS

Organska kemija / *Organic Chemistry* FFA – UN

Organska kemija / *Organic Chemistry* FFA – VS

Organska kemija / *Organic Chemistry* PEF – UN

Organska kemija / *Organic Chemistry* BF – UN

Kemija organskih materialov / *Chemistry of Organic Materials* NTF – UN

Teoretske osnove tiskarskih procesov / *Fundamental Theoretical Principles of Printing Processes* NTF – UN

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*
- Inovativna kataliza: novi procesi in selektivnost / *Innovative Catalysis: New Processes and Selectivities*
- Reakcije pod mikrovalovi in visokimi pritiski / *Microwave-Assisted Reactions and Reactions under High-Pressure*
- Študij halogeniranja organskih molekul, novi reagenti, novi pristopi / *Studies on Halogenation of Organic Compounds, New Reagents, and New Approaches*
- Raziskave reakcijskih pogojev za organske transformacije / *Studies on the Reaction Conditions for Organic Transformations*
- Priprava in uporaba imobiliziranih (polimernih) reagentov / *Preparation and Application of Immobilized (Polymeric) Reagents*
- Študij mehanizmov oksidacij organskih spojin / *Studies on the Oxidation Mechanisms of Organic Compounds*
- Študij mehanizmov fototransformacij organskih halogenidov / *Studies on the Mechanisms of Phototransformation of Halogenated Organic Compounds*
- Sinteza in karakterizacija molekularnih sond za medicinske raziskave / *Synthesis and Characterization of Molecular Probes for Medical Research*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- J. Košmrlj in A. Petrič, Nagrada Maksa Samca za popularizacijo študijev na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani za leto 2008 (skupaj z A. Pavkom) / *The Maks Samec Award for the Popularization of Studies at the University of Ljubljana, Faculty of Chemistry and Chemical Technology (together with A. Pavko)*
- D. Dolenc, Z. Kadunc in B. Šket, člani slovenskega odbora za mednarodno kemijsko olimpijado, natančneje skupine, ki usposablja tekmovalce za Mednarodno kemijsko olimpijado (MKO); Priznanje Slovenske znanstvene fundacije: Prometej znanosti za odličnost v komuniciranju za leto 2008 / *Members of the Slovenian Committee for the International Chemical Olympiad; SZF Award: Prometheus in Science for Excellence in Communication for 2008*
- A. Albreht, Prešernova nagrada FKKT za leto 2008 (mentor B. Stanovnik) / *The Faculty Prešeren Award for 2008*
- David Pahovnik, Prešernova nagrada FKKT za leto 2008 (mentor B. Stanovnik) / *The Faculty Prešeren Award for 2008*
- D. Vražič, Prešernova nagrada FKKT za leto 2008 (mentor M. Zupan) / *The Faculty Prešeren Award for 2008*

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 Nacionalni predstavnik v odboru (komiteju) Organic and Biomolecular Chemistry Division (III) IUPAC (za leti 2008–2009) / *Appointed a National Representative, IUPAC Organic and Biomolecular Division (III) Committee for the Period 2008–2009*
- B. Stanovnik je član senata za akreditacijo pri Svetu Republike Slovenije za visoko šolstvo (od 2007) / *Member of the Senate for Accreditation, The Council for Higher Education of the Republic of Slovenia (since 2007)*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- C, H, N – Analizator Perkin-Elmer 2400 II / *C, H, N – Analyzer Perkin Elmer 2400 II*
- UV – visible spektrofotometer Varian / *UV – Visible Spectrophotometer Varian*
- IR spektrometer BIO-RAD / *IR Spectrometer BIO-RAD*
- IR spektrometer Spectrum BX FTIR Perkin-Elmer / *IR Spectrometer Spectrum BX FTIR Perkin-Elmer*
- Polarimeter Perkin-Elmer / *Polarimeter Perkin-Elmer*

- Destilacijska aparatura Fisher-Jones / *Distillation Apparatus Fisher-Jones*
- Mettler-Toledo miniblock paralelni sintetizator – 12 pozicij / *Mettler-Toledo Miniblock Parallel Synthesizer – 12 Positions*
- Carousel reaction station paralelni sintetizator – 6 pozicij / *Carousel Reaction Station Paralel Synthesizer – 6 Positions*
- Büchi Syncore Polyvap+Reactor paralelni sintetizator in uparjevalnik – 24 pozicij / *Büchi Syncore Polyvap+Reactor Parallel Syntesizer and Evaporator – 24 Positions*
- Hettlab IR-Dancer Infra-Red Vortex evaporator (paralelni uparjevalnik) – 48 pozicij / *Hettlab IR-Dancer Infra-Red Vortex evaporator (parallel evaporator) – 48 positions*
- Starfish – multiexperiment work station / *Starfish – Multiexperiment Work Station*
- Laboratorijski mikrovalovni reaktor CEM / *Laboratory Microwave Reactor CEM*
- MPLC – preparativni kromatograf Büchi / *MPLC –Preparative Chromatograph Büchi*
- Aparatura za delo pod visokimi pritiski U 101 / *High-Pressure Reactor U 101*
- GC – Hewlett Packard HPG 890 Series / *GC – Hewlett Packard HPG 890 Series*
- Fotokemijski reaktor Buckinghamshire model MLU/8 / *Photochemical Reactor Buckinghamshire Model MLU/8*
- 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

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

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

TEMELJNI PROJEKTI / BASIC RESEARCH

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

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

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

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*: B. Stanovnik
Financer / *Sponsored by*: Lek d.d.

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

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

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

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – Romunija *Slovenia – Romania*	Aminokisline kot gradniki v selektivni sintezi / *Amino Acids as Building Blocks in Selective Synthesis* Nosilec / *Principal Investigator*: 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 – 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 TUJCEV NA FKKT / INVITED LECTURES AT FKKT

Prof. Domenico Spinelli, University of Bologna, Department of Organic Chemistry, *Fifty Years (or More) Playing at Opening and Closing Heterocycles: From Cusmano-Ruccia Reaction to the Discovery of Calcium Channel Modulators by a Multidisciplinar Approach*, December 2008.

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PREGLEDNI ZNANSTVENI ČLANEK / REVIEW ARTICLE

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Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
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Skalar Tina	J. Maček	2008–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

Gradiva / *Materials* – UN

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

Materiali / *Materials* – VS

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

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

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Industrijski materiali / *Industrial Materials* FMF – UN

Keramika I / *Ceramics I* NTF – UN

Gradiva / *Materials* FGG – UN in VS

Tehnologija kovin in keramike / *Technology of Metals and Ceramics* ALU – UN

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

– Raziskave in razvoj anorganskih materialov in produktov ter procesov za njihovo pripravo, materiali in kompoziti za visokotemperaturne gorivne celice, karakterizacija materialov / *Research and Develpoment of Inorganic Materials, Products and Processes for their Preparation; Materials and Composites for High Temperature Fuel Cells, Characterisation of Materials*
– Nanomateriali in nanokompoziti / *Nanomaterials and Nanocomposites*

- Industrijske odpadne snovi / *Industrial Waste Materials*
- Vpliv defektne strukture na sintranje oksidov, pretežno rutila / *Defect Structure Influence on Sintering of Oxides (Mostly Rutile)*
- Eksperimentalna verifikacija in statistična analiza veljavnosti različnih modelov procesa sintranja / *Experimetal Verification and Statistical Analysis of Different Sintering Models*
- Proučevanje procesa sintranja v prisotnosti tekoče faze ter sintranja v kemijsko heterogenih sistemih / *Study of Liquid Phase Sintering and Sintering in Heterogeneous Systems*
- Razvoj in uporaba impedančne spektroskopije za proučevanje ionskih prevodnikov in meje ionski prevodnik-kovina; znaten del aktivnosti poteka tudi na področju Li ionskih akumulatorjev / *Impedance Spectroscopy Method 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. Pejovnik, Priznanje najboljšega predavatelja na študijskem programu Kemijsko inženirstvo v študijskem letu 2007/2008 po izboru študentov / *Students Award as the Best Lecturer on Chemical Engineering Study Programme in the School Year 2007/2008*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Netzsch STA 409 aparatura za simultano termično analizo / *Apparatus for Simultaneous Thermal Analysis*
- Mettler TA 4000:
  TG 50 modul / *TG 50 Module*
  DSC 20 modul / *DSC 20 Module*
- Masni spektrometer Pfeiffer / *Mass Spectrometer Pfeiffer*
- Agilent Micro GC 3000A, plinski kromatograf / *Gas Chromatograph*
- Vrstični elektronski mikroskop Jeol T300 / *Scanning Electron Microscope Jeol T300*
- Segrevalni mikroskop Leitz Wetzlar 301-200-301 / *Heating Microscope Leitz Wetzlar 301-200-301*
- Optični mikroskop za metalografske preiskave Leitz / *Optical Microscope Leitz*

– Analizator velikosti in porazdelitve velikosti delcev Fritzsch Analysette 22 / *Particle Sizer Fritzsch Analysette 22*
– Impedančni spektrometer / *Impedance Analyser*
  1250 Frequency Response Analyser Solartron Schlumberg
  1286 Electrochemical Interface Solartron Schlumberg
– Mikroskop na atomsko silo Nanoeducator NT-MTD / *Scanning Probe Microscope Nanoeducator NT-MTD*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P–0175 Sinteza, struktura, lastnosti snovi in materialov / *Synthesis, Structure and Properties of Compounds and Materials*
Vodja programa / *Principal Researcher*: I. Leban

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

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

L2–1157 Kompoziti za litijeve baterije z veliko močjo / *Composites for High Power Lithium Batteries*
Nosilec / *Principal Researcher*: R. Dominko (KI)
Sofinancer / *Co-sponsored by*: Iskra TELA

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

– S. Pejovnik, *Moderne Li-baterije*, Univerza Đemal Bijedić, Mostar, BiH, Marec 2008
– S. Pejovnik, *Designing and Implementing HR Strategies at the Faculty Level – A Myth or Necessity*, Towards SEE Regional Competitiveness, Sofia, Bulgaria, April 2008
– S. Pejovnik, *Learning – Guidelines from the Project,* Building and Improving Support for RTD Policy and Public Spending, Istanbul, Turkey, April 2008

– S. Pejovnik, *Binding and Wiring in Advanced Battery Composites*, Workshop on Functional Nanostructures and Particles, Portorož, Slovenia, May 2008
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ATM11. MARINŠEK, Marjan. Analysis of the temperature profiles during the combustion synthesis of doped lanthanum gallate = Analiza temperaturnih profilov med zgorevalno sintezo dopiranega lantanovega galata. *Mater. tehnol.*, 2008, vol. 42, no. 2, str. 85–91. [COBISS.SI-ID 675754]

ATM12. MANDRINO, Djordje, VRBANIĆ, Daniel, JENKO, Monika, MIHAILOVIĆ, Dragan, PEJOVNIK, Stane. AES and XPS investigations of molybdenum-sulfur-iodine-based nanowire-type material. *Surf. interface anal.*, 2008, vol., no., str. [COBISS.SI-ID 513610777]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

ATM13. GOMILŠEK, Zlatko, JERMAN, Boris, NOVOSEL, Barbara. Nov pristop k vzdrževanju drogov javne in cestne razsvetljave. V: *Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož 2008, 13.–14. 5. 2008*. V Ljubljani: Fakulteta za kemijo in kemijsko tehnologijo, Oddelek za tehniško varnost, cop. 2008, str. [1–38]. [COBISS.SI-ID 29510661]

UREDNIK / EDITOR

ATM14. *Acta chimica slovenica*. Pejovnik, Stane (član uredniškega odbora 1998–). [Tiskana izd.]. Ljubljana: Slovensko kemijsko društvo: =Slovenian Chemical Society, 1993–. ISSN 1318-0207. [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

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prof. dr. Aleksander Pavko
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izr. prof. dr. Igor Plazl
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doc. dr. Ana Lakota Družina

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doc. dr. Andreja Žgajnar Gotvajn
doc. dr. Polona Žnidaršič Plazl
dr. Blaž Likozar (od 1. 11. 2008)
Urban Šegedin

Tehniki / Technicians
Klemen Birtič
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*
Gorazd Stojkovič	P. Žnidaršič Plazl	2008–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

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

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

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

Kemijsko reakcijsko inženirstvo / *Chemical Reaction Engineering* – UN

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

Biotehnologija / *Biotechnology* – UN

Pregled biokemijskih tehnologij / *Biotechnological Processes* – UN

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

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

Mehanske operacije / *Mechanical Operations* – VS

Kemijska inženirska kinetika / *Chemical Engineering Kinetics* – VS

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

Kemija okolja / *Environmental Chemistry* – UN

Ekološko inženirstvo / *Ecological Engineering* – UN

Varstvo okolja / *Environmental Engineering* – VS

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

Kemijsko procesno računstvo / *Chemical Process Calculations* – UN

Modeliranje procesov / *Process Modeling* – UN

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

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

Kemijsko inženirski praktikum / *Chemical Engineering Practice* – UN

Kemijsko inženirski praktikum / *Chemical Engineering Practice* – VS

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 – UN

Bioprocesništvo / *Bioprocess Engineering* BF – UN

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

Fizikalne, optične in kemijske metode v restavratorstvu / *Physical, Optical and Chemical Methods in Restoration* 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 (skupaj s Kemijskim inštitutom) / *Integrated Approach to Water Pollution Prevention* (*in Cooperation with the National Institute of Chemistry)*

POMEMBNI DOSEŽKI SODELAVCEV KATEDRE / SIGNIFICANT ACHIEVEMENTS OF THE CHAIR STAFF

NAGRADE IN PRIZNANJA / AWARDS, RECOGNITIONS

- T. Koloini**,** Nagrada Maksa Samca za zasluge za Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani (posthumno) / *The Maks Samec Award for the Merits for the Faculty of Chemistry and Chemical Technology, University of Ljubljana (posthumous).*
- A. Pavko**,** Nagrada Maksa Samca za popularizacijo študijev na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani (skupaj z J. Košmrljem in A. Petričem) / *The Maks Samec Award for the Popularization of Studies at the University of Ljubljana, Faculty of Chemistry and Chemical Technology (together with J. Košmrlj and A. Petrič)*
- A. Lakota Družina, priznanje najboljšega predavatelja na študijskem programu Kemijska tehnologija v študijskem letu 2007/2008 po izboru študentov / *Students Award as the Best Lecturer on Chemical Technology Professional Study Programme in the School Year 2007/2008*

ČLANSTVO V AKADEMIJAH / MEMBERSHIP IN ACADEMIES

- J. Levec, redni član Slovenske akademije znanosti in umetnosti / *Full Member, Slovenian Academy of Sciences and Arts*
- M. Berovič, član / *Member, New York Academy of Science*

ČLANSTVO V MEDNARODNIH UREDNIŠKIH ODBORIH / MEMBERSHIP IN INTERNATIONAL EDITORIAL BOARDS

- I. Plazl, *Chemical and Biochemical Engineering Quarterly*
- A. Pavko, glavni urednik / *Editor-in-Chief, Acta Chimica Slovenica*
- A. Pavko, *Food Technology and Biotechnology*
- M. Berovič, *Associate Editor, Biotechnology Annual Review*
- J. Levec, *Acta Chimica Slovenica*
- J. Levec, *Chinese Journal of Chemical Engineering*.
- J. Levec, *International Journal of Chemical Engineering*
- J. Zagorc Končan*, European Water Management*.

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

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

- Rotacijski reometer HAAKE RS 150 / *Rheometer HAAKE RS 150*
- Rotacijski reometer HAAKE CV 20 / *Rheometer HAAKE CV 20*
- UV-VIS spektrofotometer Perkin Elmer Lambda 25 / *UV-VIS Spectrophotometer Perkin Elmer Lambda 25*
- Mikrovalovni reaktor / *Microwave Reactor*
- Laboratorijski bioreaktor z mešalom / *Benchtop Fermenter Type KLF 2000*
- TOC 5000A Shimadzu aparatura / *TOC 5000A Analyser Shimadzu*
- Vary 50 Varian spektrofotometer / *Vary 50 Varian Spectrophotometer*
- Aparatura za določanje toksičnosti LUMIStox Dr. Lange / *Luminometer for Toxicity Tests LUMIStox Dr. Lange*
- Aparatura aerobni digester W11-A / *Aerobic Digester W/11-A*
- Rotacijski reometer – Physica MCR 301 / *Modular Compact Rheometer Physica MCR 301*
- Merilni sistem Protos 3400C za merjenje raztopljenega kisika / *Measuring System Protos 3400C with DO Measuring Module*

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P2–0191	Kemijsko inženirstvo / *Chemical Engineering* Vodja programa / *Principal Researcher*: M. Krajnc
P2–0150	Integralni pristop k preprečevanju onesnaževanja voda / *Integrated Approach to Water Pollution Prevention* Vodja programa / *Principal Researcher*: M. Roš (KI)

APLIKATIVNI PROJEKTI / APPLIED RESEARCH

L4–7595	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	Nadaljnja 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, tehnologije in varovanje okolja: Vpliv zamenjave kamene moke s hidra-

tiziranim 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. – Družba za avtoceste RS

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 d.d. – Družba za avtoceste RS

2/MK/2008 Razvoj novega materiala za jedro panela iz ekspandiranega perlita – faza V / *Development of New Material for Panel Core from Expanded Perlite – V*
Nosilec / *Principal Researcher*: I. Plazl
Financer / *Sponsored by*: Trimo Trebnje d.d., Trebnje

MEDNARODNO ZNANSTVENO SODELOVANJE / INTERNATIONAL RESEARCH COOPERATION

BILATERALNO MEDNARODNO SODELOVANJE / BILATERAL COOPERATION

Slovenija – 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

Mednarodno znanstveno sodelovanje med Bolgarsko akademijo znanosti in SAZU – skupni raziskovalni projekt: Implementacija mikroreaktorske tehnologije in ionskih kapljevin pri razvoju racionalnih in trajnostnih procesov biotransformacij/biodegradacij / *International Scientific Cooperation between Bulgarian Academy of Sciences and Slovenian Academy of Sciences and Arts – Joint Research Project: Implementation of Microreactor Technology and Ionic Liquids for the Development of Rational and Sustainable Biotransformation / Biodegradation Processes*.
Nosilec / *Principal Researcher*: P. Žnidaršič Plazl

VABLJENA PREDAVANJA NA INSTITUCIJAH V SLOVENIJI / INVITED LECTURES IN SLOVENIA

1. A. Zupančič Valant, N. Šegatin, Ekstrakcijske, filtracijske, separacijske tehnologije obdelave stranskih proizvodov in odpadkov živilske industrije / *Extraction, Filtration, Separation Technologies for Treatment of Co-Products and Wastes in Food Processing*, Stranski proizvodi in odpadki v živilstvu – uporabnost in ekologija, *Biotehniška fakulteta, Oddelek za živilstvo: Slovensko prehransko društvo*, Ljubljana 2008

VABLJENA PREDAVANJA NA INSTITUCIJAH V TUJINI / INVITED LECTURES ABROAD

I. Plazl, *Microreactor Technology – A New Concept in Chemical Engineering,* Universidade Téchnica de Lisboa, Departamento de Engenharia Química e Biológica, Lisboa, Portugal, June 2008

P. Žnidaršič Plazl, *Microbial Transformation of Steroid Compounds,* Faculty of Chemical Engineering and Technology, University of Zagreb, Zagreb, Croatia, March 2008

P. Plazl, *Optimization of Progesterone 11[alpha]-Hydroxylation Process Including Extraction in a Microchannel System,* The Stephan Angeloff Institute of Microbiology, Bulgarian Academy of Sciences, Sofia, Bulgaria, July 2008

VABLJENA PREDAVANJA TUJCEV NA FKKT / INVITED LECTURES AT FKKT

Prof. Dr. Blaga Angelova, The Stephan Angeloff Institute of Microbiology, Bulgarian Academy of Sciences, *Microbial Transformation of Steroid Compounds – Recent Achievements and Future Perspectives,* January 2008

BIBLIOGRAFIJA 2008 / REFERENCES 2008

IZVIRNI ZNANSTVENI ČLANEK / ORIGINAL SCIENTIFIC ARTICLE

KIŽ1. BEROVIČ, Marin, KOŠMERL, Tatjana. Monitoring of potassium hydrogen tartrate stabilization by conductivity measurement. *Acta chim. slov.*. [Tiskana izd.], 2008, letn. 55, št. 3, str. 535–540, graf. prikazi. [COBISS.SI-ID 29801733]

KIŽ2. PAVKO, Aleksander, NOVOTNÝ, Čeněk. Introduction of ligninolytic enzyme production by Dichomitus squalens on various types of immobilization support. *Acta chim. slov.*. [Tiskana izd.], 2008, letn. 55, št. 3, str. 648–652, graf. prikazi. [COBISS.SI-ID 29801989]

KIŽ3. DJINOVIĆ, Petar, BATISTA, Jurka, PINTAR, Albin. Calcination temperature and CuO loading dependence on CuO-CeO[sub]2 catalyst activity for water-gas shift reaction. *Appl. catal., A Gen.*. [Print ed.], 2008, vol. 347, no. 1, str. 23–33. [COBISS.SI-ID 3972634]

KIŽ4. PINTAR, Albin, BATISTA, Jurka, TIŠLER, Tatjana. Catalytic wet-air oxidation of aqueous solutions of formic acid, acetic acid and phenol in a continuous-flow trickle-bed reactor over Ru-TiO[sub]2 catalysts. *Appl. catal., B Environ.*. [Print ed.], 2008, vol. 84, issue 1–2, str. 30–41. [COBISS.SI-ID 3942682]

KIŽ5. DJINOVIĆ, Petar, LEVEC, Janez, PINTAR, Albin. Effect of structural and acidity/basidity changes of CuO-CeO[sub]2 catalysts on their activity for water-gas shift reaction. *Catal. today*. [Print ed.], 2008, vol. 138, no. 3/4, str. 222–227. [COBISS.SI-ID 4034586]

KIŽ6. TIŠMA, Marina, ŽNIDARŠIČ PLAZL, Polona, PLAZL, Igor, ZELIĆ, Bruno, VASIĆ-RAČKI, Đurđa. Modelling of L-DOPA oxidation catalyzed by laccase. *Chem. biochem. eng. q.*, 2008, vol. 22, no. 3, str. 307–313. [COBISS.SI-ID 29477125]

KIŽ7. LAKNER, Mitja, PLAZL, Igor. The finite differences method for solving systems on irregular shapes. *Comput. chem. eng.*. [Print ed.], 2008, vol. 32, no. 12, str. 2891–2896. [COBISS.SI-ID 29806085]

KIŽ8. DROLC, Andreja, ZAGORC-KONČAN, Jana. Diffuse sources of nitrogen compounds in the Sava River basin, Slovenia. *Desalination*. [Print ed.], Jun 2008, vol. 226, iss. 1/3, str. 256–261. [COBISS.SI-ID 3825690]

KIŽ9. COTMAN, Magda, DROLC, Andreja, ZAGORC-KONČAN, Jana. Assessment of pollution loads from point and diffuse sources in small river basin : case study Ljubljanica river. *Environmental forensics*, 2008, vol. 9, no. 2/3, str. 246–251. [COBISS.SI-ID 3980570]

KIŽ10. POHAR, Andrej, PLAZL, Igor. Laminar to turbulent transition and heat transfer in a microreactor : mathematical modeling and experiments. *Ind. eng. chem. res.*. [Print ed.], 2008, vol. 47, no. 19, str. 7447–7455. [COBISS.SI-ID 29806341]

KIŽ11. ŠVAGELJ, Mirjan, BEROVIČ, Marin, BOH, Bojana, MENARD, Anja, SIMČIČ, Saša, WRABER-HERZOG, Branka. Solid-state cultivation of Grifola frondosa (Dicks: Fr) S.F. Gray biomass and immunostimulatory effects of fungal intra- and extracellular [beta]-polysaccharides. *New biotechnology*, 2008, vol. 25, no. 2/3, str. 150–156. [COBISS.SI-ID 25058009]

KIŽ12. GREGORI, Andrej, ŠVAGELJ, Mirjan, PAHOR, Bojan, BEROVIČ, Marin, POHLEVEN, Franc. The use of spent brewery grains for Pleurotus ostreatus cultivation and enzyme production. *New biotechnology*, 2008, vol. 25, no. 2/3, str. 157–161. [COBISS.SI-ID 30014981]

KIŽ13. BEROVIČ, Marin, POTOČNIK, Mateja, ŠTRUS, Jasna. The influence of galvanic field on Saccharomyces cerevisiae in grape must fermentation. *Vitis*, 2008, vol. 47, no. 2, str. 117–122, graf. prikazi. [COBISS.SI-ID 29745157]

KIŽ14. ŽGAJNAR GOTVAJN, Andreja, ZAGORC-KONČAN, Jana, DERCO, Ján, ALMÁSIOVÁ, Beáta, KASSAI, Angelika. Oxidative pretreatment of fresh and mature landfill leachate. *Journal of advanced oxidation technologies*, 2009, vol. 12, no. 1, str. 1–10, graf. prikazi. [COBISS.SI-ID 30047493]

KIŽ15. ŽGAJNAR GOTVAJN, Andreja, TIŠLER, Tatjana, ZAGORC-KONČAN, Jana. Comparison of different treatment strategies for industrial landfill leachate. *J. hazard. mater.*. [Print ed.], 2009, vol. 162, no. 2/3, str. 1446–1456. [COBISS.SI-ID 29958149]

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

KIŽ16. BEROVIČ, Marin, BOH, Bojana, WRABER-HERZOG, Branka. Production of pharmaceutically active compounds of Grifola frondosa by solid state and submerged cultivation : [plenary lecture]. V: *International conference on technologies and strategic management of suistanable biosystems*. [S. l.: s. n.], 2008, [1–9] str., graf. prikazi. [COBISS.SI-ID 29746437]

KIŽ17. ZUPANČIČ-VALANT, Andreja, ŠEGATIN, Nataša. Ekstrakcijske, filtracijske, separacijske tehnologije obdelave stranskih proizvodov in odpadkov živilske industrije = Extraction, filtration, separation technologies for treatment of co-products and wastes in food processing. V: GAŠPERLIN, Lea (ur.), ŽLENDER, Božidar (ur.). *Stranski proizvodi in odpadki v živilstvu – uporabnost in ekologija*. Ljubljana: Biotehniška fakulteta, Oddelek za živilstvo: Slovensko prehransko društvo, 2008, str. 85–94. [COBISS.SI-ID 3427960]

OBJAVLJENI ZNANSTVENI PRISPEVEK NA KONFERENCI / PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

KIŽ18. LAKOTA, Ana. Analysis of experimental gas holdup data from a cocurrent upflow bubble column operating with xanthan solutions. V: 18th International Congress of Chemical and Process Engineering, 24–28 August 2008, Praha, Czech Republic. *CHISA 2008 : CD-ROM of full texts*. Praha: Czech Society of Chemical Engineering, 2008, [1–8] str., graf. prikazi. [COBISS.SI-ID 29755397]

KIŽ19. ŽNIDARŠIČ PLAZL, Polona, POHAR, Andrej, PLAZL, Igor. Lipase-catalyzed isoamyl acetate synthesis in a microreactor with ionic liquid as a reaction medium. V: 18th International Congress of Chemical and Process Engineering, 24–28 August 2008, Praha, Czech Republic. *CHISA 2008 : CD-ROM of full texts*. Praha: Czech Society of Chemical Engineering, 2008, [1–8] str., graf. prikazi. [COBISS.SI-ID 29755141]

KIŽ20. TIŠLER, Tatjana, ZAGORC-KONČAN, Jana. Toxicity assessment of effluents. V: KUNGOLOS, Athanassios (ur.). *Environmental toxicology II*, (WIT transactions on ecology and the environment, vol. 110). Southampton: WIT Press, 2008, str. 83–91. [COBISS.SI-ID 3949338]

KIŽ21. COTMAN, Magda, ŽGAJNAR GOTVAJN, Andreja. Toxicity reduction evaluation (TRE) procedure for identification of toxic substances in landfill leacdhate. V: KUNGOLOS, Athanassios (ur.). *Environmental toxicology II*, (WIT transactions on ecology and the environment, vol. 110). Southampton: WIT Press, 2008, str. 117–126. [COBISS.SI-ID 3949594]

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PUMA

KATEDRA ZA POLIMERNO INŽENIRSTVO, ORGANSKO KEMIJSKO TEHNOLOGIJO IN MATERIALE
CHAIR OF POLYMER ENGINEERING, ORGANIC CHEMICAL TECHNOLOGY AND MATERIALS

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SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
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doc. dr. Urška Šebenik

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Branko Alič, univ. dipl. kem.

Tehnik / Technician
Janez Malovrh

Mladi raziskovalci *Young Researchers*	Mentor *Mentor*	Čas usposabljanja *Programme Duration*	Oblika usposabljanja *Degree*
Blaž Likozar	M. Krajnc	2004–2009	doktorski študij / *PhD*
Jošt Mohorko	M. Krajnc	2005–2008	magistrski študij / *MSc*
Sašo Rogelj	M. Krajnc	2003–2008	doktorski študij / *PhD*
Jernej Kajtna	J. Golob	2003–2008	doktorski študij / *PhD*
Maja Šoštarič	J. Golob	2007–2012	doktorski študij / *PhD*
Ines Mohorič	U. Šebenik	2008–2013	doktorski študij / *PhD*

IZOBRAŽEVALNA IN RAZISKOVALNA DEJAVNOST KATEDRE / EDUCATIONAL AND RESEARCH ACTIVITIES

IZOBRAŽEVALNA DEJAVNOST / LECTURED COURSES

FKKT / FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Dodiplomski programi / *Undergraduate Programmes*

- Pregled tehnologij / *Principles of Technological Processes* – UN
- Uvod v tehnologijo / *Introduction to Technology* – VS
- Organski procesi in produkti / *Organic Processes and Products* – VS
- Osnove kemijskih tehnoloških procesov / *Fundamentals of Technological Processes* – UN
- Organska tehnologija I / *Organic Chemical Technology I* – UN
- Polimeri / *Polymers* – UN
- Separacijski procesi / *Separation Processes* – UN
- Organski materiali in produkti / *Organic Materials and Products* – UN

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*

IZVEN FKKT / EXTRAMURAL COURSES

Dodiplomski programi / *Undergraduate Programmes*

- Polimerni materiali / *Polymer Materials* BF – UN
- Polimerna kemija / *Polymer Chemistry* NTF – UN

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

- Študij kinetike med vulkanizacijo različnih gumenih zmesi / *Kinetic Investigations During Vulcanization Proceses of Different Rubber Blends*
- Študij prenosa toplote med vulkanizacijo različnih gumenih zmesi / *Heat Transfer Investigations During Vulcanization Proceses of Different Rubber Blends*
- Testiranje mehanskih lastnosti gume in gumenih kompozitov / *Testing of Rubber and Rubber Composites*
- Sinteza, karakterizacija in optimizacija procesa sinteze fenol-formeldehidnih smol, sečninsko-formaldehidnih smol, melaminsko-formaldehidnih smol, fenol-sečninsko-formaldehidnih smol, melamin-sečninsko-formaldehidnih smol / *Synthesis, Characterization and Synthesis Process Optimization of Formaldehyde Resins*

- Tehnologija priprave melamiskih pen / *Technology for the Production of Melamine Foams*
- Enkapsulacija / *Encapsulation*
- Polisiloksanske emulzije na vodni osnovi / *Polysiloxane water-based emulsions*
- Sinteza, karakterizacija in optimizacija procesa sinteze akrilatnih lepil / *Synthesis, Characterization and Synthesis Process Optimization of Acrylic Adhesives*
- Sinteza, priprava in karakterizacija nanokompozitnih materialov / *Synthesis, Preparation and Characterization of Nanocomposite Materials*
- Raziskave na področju ekspanzijskega injekcijskega stiskanja / *Research in the Field of Injection Blow Molding*
- 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

NAGRADE, PRIZNANJA / AWARDS, RECOGNITIONS

- J. Kajtna, Nagrada Maksa Samca za najboljši doktorat (mentor J. Golob, somentor M. Krajnc) / *The Maks Samec Award for the Best PhD Thesis*

RAZISKOVALNA OPREMA / RESEARCH EQUIPMENT

- Mettler Toledo DMA 861e
- Mettler Toledo DSC 821e
- Mettler Toledo ReactIR iC10
- Perkin Elmer FTIR Spectrum 1000
- HP 5980II Gas Chromatograph
- LC Shimadzu LC-4A
- Microtrac S 3500 Laser Particle Size Analyzer
- Extruder Brabender Plasticorder PLD 651
- 3D-DLS Research Lab
- Mettler Toledo LabMax Automatic Lab Reactor

SODELOVANJE V TEHNOLOŠKIH MREŽAH IN PLATFORMAH / TECHNOLOGY NETWORKS & PLATFORMS

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

RAZISKOVALNI PROGRAMI IN PROJEKTI / RESEARCH PROGRAMMES AND PROJECTS

RAZISKOVALNI PROGRAMI / RESEARCH PROGRAMMES

P2–0191 Kemijsko inženirstvo / *Chemical Engineering*
Vodja programa / *Principal Researcher*: M. Krajnc

RAZVOJNI PROJEKTI / INDUSTRIAL RESEARCH AND DEVELOPMENT

Enkapsulacija / *Encapsulation*
Nosilec / *Principal Researcher*: M. Krajnc
Financer / *Sponsored by*: Melamin d.d.

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

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

Biodiesel / *Biodiesel*
Nosilec / *Principal Researcher*: J. Golob
Financer / *Sponsored by*: Nafta Petrochem d.o.o.

Oplaščanje umetnih gnojil s podaljšanim delovanjem, sinteza kelatov in adsorpcija biocidov v praškastih formulacijah za agrokemijske namene / *Preparation of Polymer-Coated Controlled-Release Fertilizers, Chelate Synthesis, and Study of Biocide Adsorption in Powder Formulations for Agrochemical Purposes*
Nosilec / *Principal Researcher*: J. Golob
Financer / *Sponsored by*: Unichem d.o.o.

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KATEDRA ZA VARSTVO PRI DELU
CHAIR OF SAFETY AT WORK

PREDSTOJNIK KATEDRE / HEAD

dr. Jože Šrekl

SODELAVCI KATEDRE / PERSONNEL

Učitelji / Faculty
dr. Mitja Robert Kožuh, viš. pred.
dr. Jože Šrekl, viš. pred.
mag. Aleš Jug, pred.
prof. dr. Stojan Petelin (v dopolnilnem razmerju)
doc. dr. Marija Molan (v dopolnilnem razmerju)

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* – VS

Tehniška mehanika / *Technical Mechanics* – VS

Računalništvo / *Computer Science* – VS

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

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

Varstvo okolja I / *Environmental Protection I* – VS

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

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

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

Psihologija dela / *Occupational Psychology* – VS

Varstvo okolja II / *Environmental Protection II* – VS

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

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

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

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

RAZISKOVALNA DEJAVNOST / RESEARCH ACTIVITIES

- Nove metodologije ocenjevanja tveganja / *New Methods in Risk Assessment*
- Ocenjevanje kompleksnih tehnoloških sistemov / *Assessment of Complex Techological Systems*
- Človek – element tveganja / *Human as a Risk Factor*
- Metodologija statistike požarov /*Methodology of Fire Statistics*
- Inženirske metode pri vrednotenju požarne varnosti / *Engineering Methods in Fire Safety Assessment*
- Modeliranje s strukturnimi enačbami v oceni požarne ogroženosti / *Structural 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

– Ančka Gantar, Nagrada Avgusta Kuharja za najboljše diplomsko delo za leto 2008 / *The Avgust Kuhar Award for the Best Diploma Work for 2008*
– J. Jerman, priznanje najboljšega predavatelja na študijskem programu Tehniška varnost v študijskem letu 2007/2008 po izboru študentov / *Students Award as the Best Lecturer on Safety at Work Study Programme in the School Year 2007/2008*

ORGANIZACIJA MEDNARODNIH SREČANJ / ORGANISATION OF INTERNATIONAL MEETINGS

– Varstvo pri delu, varstvo pred požari in medicina dela : dvodnevni posvet z mednarodno udeležbo, Portorož, maj 2008 / *Safety at Work, Fire Safety and Occupational Medicine, Two Days Symposium with International Participation, Portorož, May 2008*

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 d.d. – Družba za avtoceste 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

Oba projekta sta bila v letu 2008 zaključena.

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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