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Annual report 2006

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Ljubljana, 2007

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Govor direktorja na slovesnosti ob 60. obletnici Kemijskega inštituta

Speech of the Director at the Celebration of the 60th Anniversary of the National Institute of Chemistry

Ljubljana, 29. maj, 2007

Kemijski inštitut je bil vse od skromnih začetkov pod vodstvom profesorja Maksa Samca pa vse do danes zvest svojemu poslanstvu in osnovnim vrednotam, ki so: odlična znanost in sodelovanje z gospodarstvom, čemur se vse bolj intenzivno pridružuje tudi kakovostno izobraževanje. V 60. letih od svoje ustanovitve se je inštitut razvil v moderno, dobro opremljeno raziskovalno ustanovo, ki je vpeta v globalne raziskovalne tokove s ciljem, da čim bolj prispeva k gospodarskemu napredku in izboljševanju kvalitete življenja v Sloveniji.

V nadaljevanju se bom osredotočil na izvajanje osnovnih strateških ciljev inštituta v obdobju zadnjih desetih let.

Kemijski inštitut stalno povečuje nivo znanja in znanosti na področjih:

- biotehnologije in kemije zdravil (tudi prehrane),
- materialov in inženirstva,
- varstva okolja in analize kemije ter
- strukturne in računalniške kemije.

Ljubljana, May 29, 2007

The National Institute of Chemistry (NIC) has been, from its very beginnings under the leadership of Professor Maks Samec until today, true to its mission and fundamental values, which are: high-level science and cooperation with industry, to which high-quality education is ever more strongly linked. In the 60 years since its establishment, the NIC has developed into a modern, well-equipped research institution, which is a part of global research efforts, with the aim of aiding the economic advancement and enhancing the quality of life in Slovenia.

Now, let us focus on the implementation of the fundamental strategic goals of the NIC within the past 10 years.

NIC has consistently raised the level of understanding and science in the fields of:

- biotechnology and the chemistry drugs (as well as food),
- materials and engineering,
- environmental protection and analytical chemistry, as well as
- structural and computational chemistry.

Vse večjo kvaliteto raziskav sodelavcev Kemijskega inštituta potrjujejo objave v vse boljših znanstvenih revijah, na kar kaže na primer rast povprečnega faktorja vpliva revij v katerih objavljamo znanstvene članke. Za kvalitetno raziskovalno delo je izjemno pomembno mednarodno sodelovanje in naše uspešno konkuriranje za evropske in druge mednarodne raziskovalne projekte. K temu veliko pripomore naša tradicionalna odprtost v mednarodni prostor in strokovno delo naših raziskovalcev med gostovanjem na najprestižnejših institucijah v tujini, kjer so vedno dobrodošli. Za raziskave, primerljive z najboljšimi v svetu je poleg zagnanih znanstvenikov potrebna tudi ustrezna raziskovalna oprema in pogoji dela. Tudi v zadnjem obdobju smo zato vložili veliko energije v investicije. Med drugim smo izpeljali tudi največjo investicijo v posamezno raziskovalno opremo v Sloveniji, 800 MHz NMR spektrometer, ki skupaj z drugimi instrumenti v našem evropskem centru odličnosti predstavlja pomembno evropsko raziskovalno infrastrukturo. Vse večji interes znanstvenikov iz tujine za raziskovalno delo na našem inštitutu je dober pokazatelj, da smo na pravi poti. Na dobro primerljivost z najboljšimi na svetu pa je pokazala tudi primerjalna študija evropskih raziskovalnih inštitutov iz leta 2002, kjer smo kljub skromnejšim finančnim virom presegali ostale evropske inštitute po mnogih kriterijih.

Ena izmed stalnic, ki spremlja naš inštitut že vse od ustanovitve, je nedvomno intenzivno sodelovanje z gospodarstvom. Kemijski inštitut vseskozi veliko in uspešno sodeluje s podjetji. To sodelovanje od nas zahteva veliko urejenost našega dela in poslovanja, ter nam obenem omogoča pridobivanje dodatnih znanj in finančnih sredstev, s katerimi lahko kupujemo za dolgoročni razvoj inštituta nujno potrebno raziskovalno opremo. S podjetji v Sloveniji smo vzpostavili mnoga dolgoročna partnerstva, ki temeljijo na visoki stopnji medsebojnega zaupanja, kar smo mnogokrat okrepiли tudi z izmenjavo strokovnjakov.

The ever higher quality of the research of those working at the NIC is shown by the increase in publications in better scientific journals, it is also evidenced by the higher impact factors of the journals where our scientific articles are published. International cooperation is very important in order to carry out high-quality research work and for our successful competition for European and other international research projects. To this end, our traditional openness in the international sphere and the professional work of our researchers while visiting prestigious institutions abroad, where they are always welcome, has helped us. For research, to be comparable with the best in the world, there cannot be simply enthusiastic scientists, but there must also be appropriate research equipment and working conditions. Within the past few years, we have put a lot of energy into investment. Among other things, we have made the largest investment into an individual piece of research equipment in Slovenia in the form of an 800 MHz NMR spectrometer, which, together with other instruments in our European Centre of Excellence, represents an important part of Europe's research infrastructure. There is an ever greater interest from abroad in undertaking research work at the NIC, which is a good sign that we are heading in the right direction. A comparative study of European research institutes from 2002 showed the NIC to be quite competitive with the best in the world, as we managed, despite more modest financial resources, to outdo other European institutions on many criteria.

One of the constants which has been with our institute from its foundation is the strong cooperation with industry. The NIC has consistently cooperated in a large-scale and successful way with companies. This cooperation has demanded a great deal of organization in our work and business matters, but at the same time has allowed us to obtain additional knowledge and financial resources, with which we have been able to buy research equipment for the long-term development of the institute. We have also created a number of long-term part-



Obleženje 60. obletnice Kemijskega inštituta, Grand Hotel Union, Ljubljana, 29. maj 2007

Celebration of the 60th anniversary of the National Institute of Chemistry, Grand Hotel Union, Ljubljana, May 29, 2007

Zato smo na Kemijskem inštitutu zelo zadovoljni ob izredno uspešnem razvoju naših gospodarskih partnerjev, saj se nekateri od njih uvrščajo med največja in najuspešnejša slovenska podjetja; med tista, ki delujejo globalno in se uspešno soočajo s svetovno konkurenco. Zavedamo se, da bomo lahko uspešno sodelovali in pripomogli k njihovi uspešnosti tudi v prihodnje le tako, da bo tudi naše znanje globalno konkurenčno. Povprečno znanje ali znanost enostavno nista dovolj dobra! Vse več Kemijski inštitut sodeluje tudi s podjetji iz tujine, podjetniške izkušnje pa pridobivamo tudi s soustanovitvijo podjetja na Nizozemskem, na področju kemometrije skupaj z nekaterimi odličnimi tujimi raziskovalnimi ustanovami. Ilustracija naše inovativnosti je uspešen preboj izuma inštituta na področju prehranskih dopolnil, ki nam je uspel skupaj z industrijskim partnerjem.

Odličen nivo znanja, podkrepjen z ustreznimi pogoji dela ter sodobno raziskovalno infrastrukturo pa ni le nujen pogoj za uspešno sodelovanje z gospodarstvom in za doseganje odlične znanosti v mednarodnih okvirih, ampak je tudi nujen pogoj za postavitve kvalitetnega izobraževanja. Kemijski inštitut uspešno sodeluje tudi v procesih izobraževanja. V obdobju zadnjih desetih let je raziskovalno delo za doktorsko disertacijo opravilo 74 raziskovalcev, za magisterij 42 raziskovalcev, raziskovalno delo za diplomsko delo pa kar 323 študentov. Trenutno na inštitutu opravlja svoje raziskovalno delo kar 65 doktorskih študentov, približno ena tretjina (od 96) doktorjev znanosti pa je habilitiranih na slovenskih univerzah. Na našo uspešno sodelovanje pri izobraževanju kaže tudi odmevna mednarodna zmaga na tekmovanju študentov najboljših svetovnih univerz iz področja sintezne biologije v lanskem letu.

Glede na doseženo, ni presenetljivo, da smo v postopku ustanovitve visokošolskega zavoda Raziskovalne šole Kemijskega inštituta. Prepričani smo, da v strateškem partnerstvu z drugimi

nerships with companies in Slovenia, which are based on a high-level of interpersonal trust and have been strengthened through exchanges of experts.

Therefore, the NIC is very pleased with the exceptionally successful development of our economic partners, many of whom are among the largest and most successful in Slovenia, even among those who do business globally and must therefore face tough global competition. We are aware that we can successfully cooperate and also contribute to their success in the future only if our own knowledge is globally competitive. Average knowledge or science is simply not good enough! The NIC is working more and more with foreign companies. We are also gaining business experience through the co-establishment of a company in the Netherlands in the field of chemometrics, together with other high-level research institutions. An illustration of our innovativeness has been the breakthrough invention of our institute in the field of nutritional supplements in cooperation with industrial partners.

An excellent level of knowledge strengthened by appropriate working conditions and a modern research infrastructure are not the only necessary conditions for successful cooperation with industry and for achieving excellent science in an international framework, another necessary condition needed is high-quality education. The NIC successfully participates in the education process. Within the past ten years, research work at the NIC towards a PhD was completed by 74 researchers, towards a Master's degree by 42 researchers, and towards a B.S. degree by 323 students. At the moment, 65 doctoral students are undertaking research work at the institute and approximately one-third (out of 96) of our PhD's are affiliated with a university. Our successful association with education is also shown by the amazing win by a Slovenian group at an international competition of students from the world's best universities in the field of synthetic biology last year.

visokošolskimi organizacijami lahko prispevamo h globalni konkurenčnosti slovenskega visokošolskega izobraževanja in posredno tudi konkurenčnosti slovenskega gospodarstva.

Za uspešno tekmo na svetovnem nivoju v prihodnje, bomo morali še bolje povezati vse naše sposobnosti in znanja tako na inštitutu kot tudi širše v Sloveniji. V teh procesih bo velika priložnost inštituta njegova interdisciplinarnost. Raziskovalci, ki delajo na Kemijskem inštitutu, prihajajo s področij kemije, fizike, biologije, farmacije, medicine in matematike. Prepričan sem, da bo prav bolje usklajeno delo posameznikov in manjših skupin z različnih raziskovalnih področij pomembno prispevalo k uspešnemu sodelovanju tudi v globalno zelo konkurenčnih raziskovalnih projektih. Nekaj takšnih mednarodnih projektov, kjer sodeluje več raziskovalnih skupin inštituta je že v teku. Na primer omenjeni NMR Center, projekt gorivnih celic ter projekt nanobiofarmacevtike.

Kemijski inštitut je v 60. letih prehodil izredno uspešno pot. K temu so s svojim ustvarjalnim delom največ prispevali prav sodelavci inštituta. Lepa hvala vsem za vaš prispevek k razvoju inštituta. Meni osebno pa je v veselje, da sem lahko sodeloval z vami in tako po svojih močeh prispeval k razvoju našega inštituta.

Mnoge uspešne projekte pa nismo izpeljali sami, ampak skupaj s partnerji iz akademske sfere in gospodarstva. Zato se želim ob koncu zahvaliti vsem našim partnerjem za uspešno sodelovanje z upanjem, da ga v prihodnjih letih še okrepimo.

With all we have achieved it is no surprise that we are in the process of establishing an institute of higher education: the Research School of the National Institute of Chemistry. We are convinced that in a strategic partnership with other organizations of higher education we can contribute to the global competitiveness of Slovenian higher education and, indirectly, to the competitiveness of the Slovenian economy as a whole.

In order to successfully compete on a global level in the future we are going to have to bring together all of our knowledge and capabilities not only within the institute but also within Slovenia itself. The interdisciplinary nature of the NIC will be a great advantage in this regard. Researchers who work at the institute come from the fields of chemistry, physics, biology, pharmacy, medicine, and mathematics. I am convinced that closer work between individuals and smaller groups from different fields of research will also contribute to successful collaboration in highly competitive research projects. Such international projects, where many research groups from the NIC are already participating, are currently up and running, for example, the previously mentioned NMR Center, a fuel cell project and a project concerning nanobiopharmaceuticals.

The National Institute of Chemistry has travelled a remarkably successful road over the past 60 years. Those who have worked at the institute have contributed to this success through their own creative work. Thank you all for your contribution to the development of the institute. I am personally very pleased to have been able to work with you and to contribute my own talents to the development of the institute.

Many successful projects have not been carried out by us alone, but together with partners from the academic sphere and the economy. Therefore, I would finally like to thank all of our partners for their successful partnerships with the hope that these will only be strengthened in the future.

Govor predsednika vlade Republike Slovenije, gospoda Janeza Janše, na slovesnosti ob 60. obletnici Kemijskega inštituta

Speech of the Prime Minister of the Republic of Slovenia Mr. Janez Janša at the Celebration of the 60th Anniversary of the National Institute of Chemistry

Ljubljana, 29. maj, 2007

Spoštovani!

Znanost in tehnologija postavljata meje našega življenja vedno znova na preizkušnjo. Ali kakor je nekoč dejal Goethe: » Človek mora neprestano verjeti, da je nedoumljivo doumljivo, sicer ne bi ničesar odkril.«

Tako so stvari, ki si jih včasih nismo upali niti zamisliti, danes nekaj vsakdanjega, pogledi znanstvenikov in raziskovalcev pa so že usmerjeni v prihodnost, onstran znanega in možnega.

Danes imamo na razpolago več znanja in tehnologije kot pred 60. leti, ko je bil ustanovljen Kemijski inštitut.

V času od ustanovitve pa do danes se je spremenilo mnogo - ljudje, zgradba, oprema, raziskovalne metode, vendar sta glavni »kemijski« sestavini, to sta ljubezen do kemije in želja po njenem raziskovanju, ostali. V tem času je inštitut postal doma in v svetu prepoznavna raziskovalna organizacija na področju kemije in sorodnih disciplin. S svojim raziskovalnim delom in sodobno infrastrukturo

Ljubljana, May 29, 2007

Ladies and Gentlemen!

Science and technology have put the limits of our lives to a test over and over again. Or as Goethe once said: Man must always believe that the unknown can be understood, otherwise nothing can be discovered. Things that we did not even dare imagine in the past are now common in our every day, while the eyes of scientists and researchers are already looking into a future beyond the known and possible.

Today we have available more knowledge and technology than 60 years ago when the National Institute of Chemistry was established. In the time since its establishments many things changed – the people, the building, the equipment, the research methods – however, two main »chemical« ingredients remain: the love for chemistry and a wish to research it. Over this period the institute has grown into a well respected institution in the area of chemistry and related sciences in Slovenia and around the world. With its reaserch and modern infrastructure it today ensures top science and research

zagotavlja danes vrhunske znanstveno-raziskovalne dosežke, vzgojo kadrov in prenos novih znanj v gospodarstvo.

V teh 60-ih letih delovanja pa se ni spremenil samo inštitut, ampak tudi naša država in njen gospodarski položaj, ki nam danes omogoča, da si zastavimo višje in bolj ambiciozne cilje, saj nas le drznost, znanje in ustvarjalnost lahko dvigneta iz povprečja. Slovenija postaja ustvarjalno okolje za ljudi, ki imajo zamisli in energijo, da jih uresničijo. Naj bo to naša primerjalna prednost pred drugimi tudi v prihodnje. Potrebno je namreč ustvariti pogoje za ohranitev in pritegnitev najodličnejših strokovnjakov, kar je ključni izziv Slovenije in Evropske unije, zato velja pozdraviti uspešno sodelovanje Kemijskega inštituta v evropskih projektih, sodelovanje z domačimi in tujimi univerzami in industrijo ter mobilnost raziskovalcev.

Slovenija si je na področju raziskav in razvoja zastavila ambiciozne cilje, ti so zapisani v Resoluciji o nacionalnem raziskovalnem in razvojnem programu za obdobje do leta 2010. V njej se je zavezala k povečanju vpliva raziskav in razvoja v Sloveniji, k povečanju vlaganj v ta sektor ter k dvigu kakovosti našega raziskovalnega sistema tako s spodbujanjem razvoja človeških virov, kot tudi s spodbujanjem primerne okolja za razvoj raziskovalnih institucij in visokotehnoških podjetij. Za razvojne premike pa so potrebni dolgoročni napori celotne družbe. Rezultati se ne pokažejo takoj. Slovenija je trdno odločena, da se je na znanju temelječ razvoj naše družbe, ki ga smiselno podpira tudi sedmi okvirni program raziskav in tehnološkega razvoja Evropske unije, edina prava in možna pozitivna prihodnost.

Zelo me veseli, da ste na Kemijskem inštitutu željo po prispevku h gospodarskem napredku in izboljšanju kvalitete življenja, jasno zapisali v svoje poslanstvo. Zlasti velja pozdraviti vaš posluš za mlade, še posebej študente, saj jih je lepo število vključeno v program mladih raziskovalcev.

results, the education of professionals, and the transfer of knowledge into the economy.

In the 60 years of its existence it was not only the institute that changed, but our country as well. We now have a different economic position that allows us to set our goals higher and to be more ambitious, since only daring, knowledge and creativity can raise us above the average. Slovenia is becoming a creative environment for people that have ideas and the energy to make them come true. This should be our comparative advantage in the future as well. It is necessary that we create conditions that will allow us to retain and attract the most prominent experts, a key challenge for both Slovenia and the European Union. Therefore we can be pleased with the successful involvement of the National Institute of Chemistry in European projects, its cooperation with domestic and foreign universities and industry, and the mobility of its researchers.

In research and development Slovenia has set itself ambitious goals as written into the Resolution on the National Research and Development Program for the period up to 2010. In it, Slovenia has made a commitment to increase the influence of research and development, to increase the investment in this sector, and to raise the quality of our research system both by support for the development of human resources as well as by creating an adequate environment for the development of research institutions and high technology companies. A significant development movement however requires longterm efforts on the part of the whole society. The results will not be seen immediately. Slovenia is determined that knowledge based development, supported by the seventh research and technology development framework program of the European Union, is the only true and possible positive future.

It is therefore a pleasure to see that at the National Institute of Chemistry you chose to clearly set out your contribution to Slovenian economic development and the improvement in the qual-

Suverenost človeka je v znanju, zato si želimo, da bi se Kemijski inštitut še bolj intenzivno vključil v programe spodbujanja mladih za študij naravoslovja in tehnike, svoje raziskovalce pa ponudil kot mentorje osnovnošolcem in srednješolcem ter njihovim profesorjem.

ity of life into your mission statement. Most encouraging is your care for young researchers, especially for students, which can be seen from the number of those included in the young researchers program. The sovereignty of a human is in his knowledge and we want the National Institute of Chemistry to become even more involved in the programs designed to promote the study of natural sciences and technology and offer its researchers as mentors to elementary and high school students and their professors.



Predsednik Vlade Republike Slovenije, gospod Janez Janša, je imel slavnostni nagovor

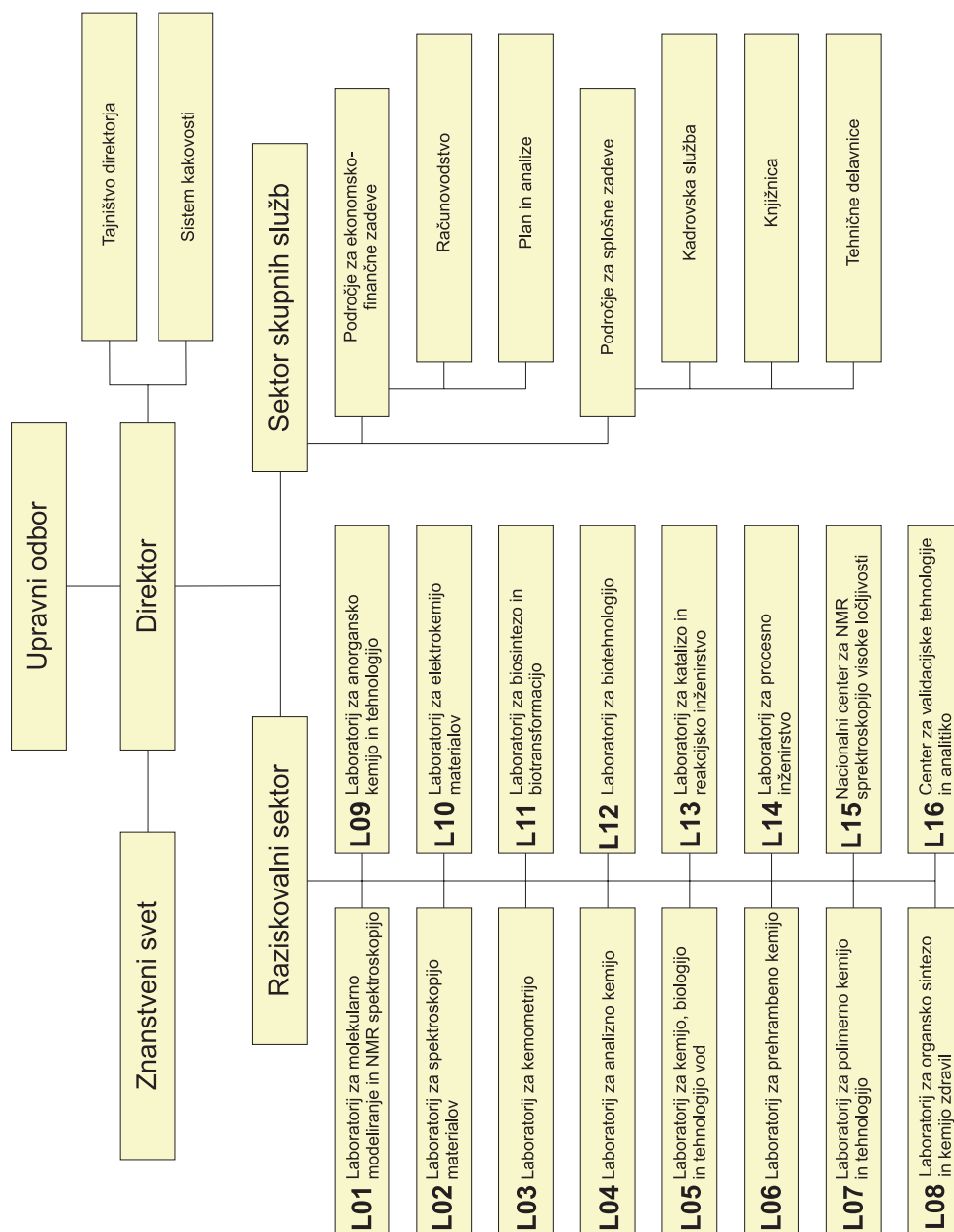
The Prime Minister of the Republic of Slovenia Janez Janša during his address

Poslanstvo Kemijskega inštituta

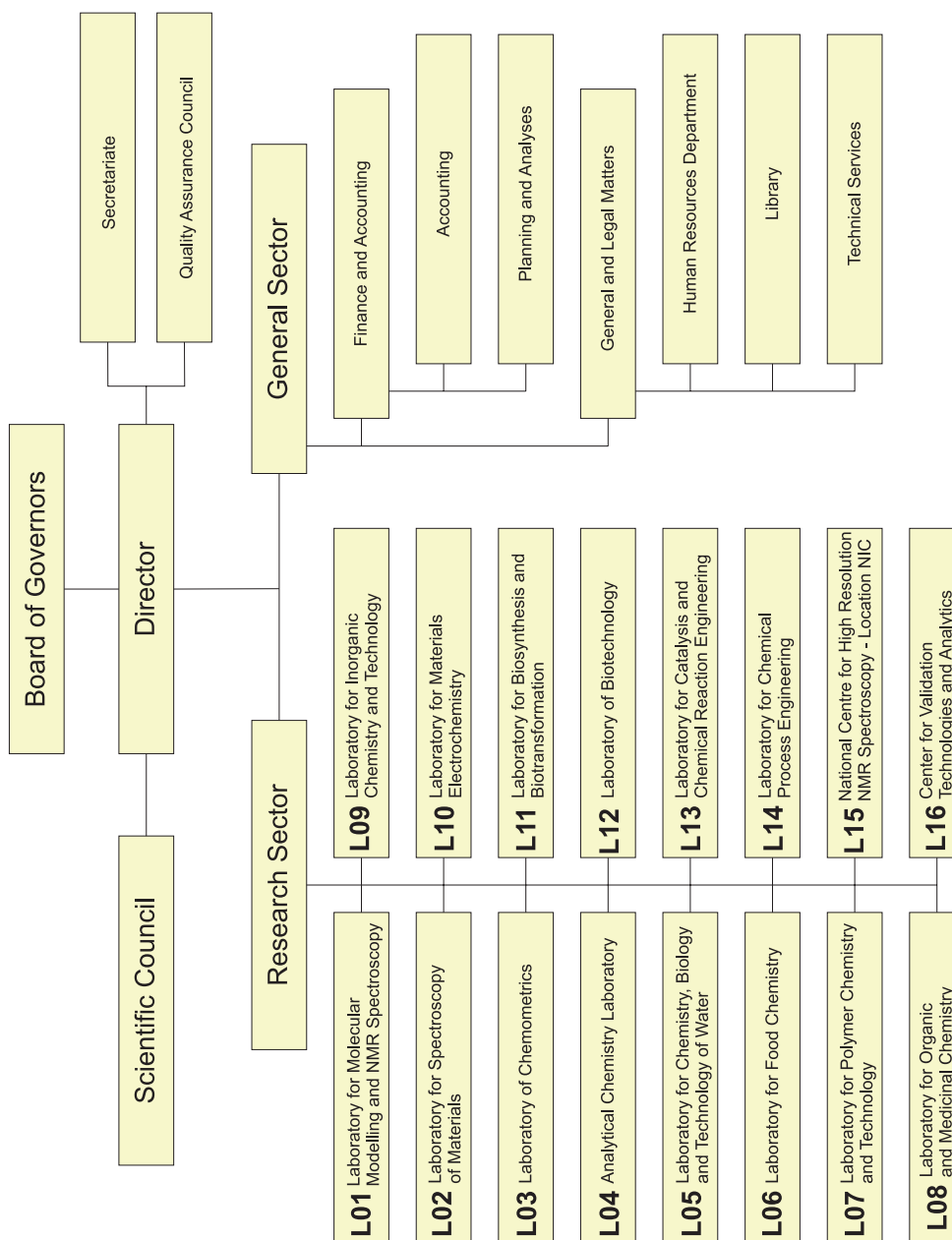
The Mission of the National Institute of Chemistry

- Kemijski inštitut je v Sloveniji vodilna in v svetu prepoznavna raziskovalna organizacija na področju kemije in sorodnih disciplin.
- Z raziskovalnim delom in moderno infrastrukturo zagotavlja vrhunske znanstveno - raziskovalne dosežke, vzgojo kadrov in prenos novih znanj v gospodarstvo.
- Kemijski inštitut s svojim delom pomembno prispeva h gospodarskemu napredku in izboljšanju kakovosti življenja v Sloveniji.
- The National Institute of Chemistry is Slovenian leading and worldwide known research institution in the field of chemistry and related disciplines.
- Performed research and modern infrastructure enables top-level scientific research achievements, nurturing new human potentials and transferring knowledge into the economy.
- The results of National Institute of Chemistry substantially contribute to the economic growth and improvement of quality of life in Slovenia.

Organizacijska shema



Organisation Chart



Vodstvo inštituta

Institute Management

VODSTVO / MANAGEMENT

- **Direktor / Director**
Doc. dr. Peter VENTURINI
- **Pomočniki direktorja / Assistant directors**
Mag. Janez TOPLIŠEK (do avgusta / until august 2006)
Andreja VRAN (od septembra / since september 2006)
Mag. Renata VUGA
- **Svetovalec direktorja / Councillor to the director**
Doc. dr. Janko ŽMITEK

ČLANI UPRAVNEGA ODBORA / BOARD OF GOVERNORS

- Dr. Matej Penca, predsednik / president
- Dr. Zvonko Bergant (do / until 20. 4. 2006)
- Prof. dr. Roman Jerala
- Dr. Gregor Gomišček (od / since 20. 4. 2006)
- Akad. prof. dr. Dušan Hadži (do / until 20. 4. 2006)
- Doc. dr. Andrej Kitanovski (od / since 20. 4. 2006)
- Prof. dr. Julijana Kristl (do / until 20. 4. 2006)
- Dr. Andrej Kržan
- Dr. Brina Ornik
- Doc. dr. Janez Plavec
- Božo Šest (od / since 20. 4. 2006)
- Prof. dr. Tomaž Šolmajer

ČLANI ZNANSTVENEGA SVETA / SCIENTIFIC COUNCIL

- Doc. dr. Janez Jamnik, predsednik / president
- Dr. Franc Avbelj
- Prof. dr. Branko Borštnik
- Prof. dr. Roman Jerala
- Prof. dr. Venčeslav Kaučič
- Dr. Albin Pintar
- Doc. dr. Janez Plavec
- Prof. dr. Milenko Roš
- Izr. prof. dr. Majda Žigon
- Doc. dr. Peter Venturini, direktor (član po funkciji / member by function)

ČASTNI ČLANI / HONORARY MEMBERS

- Prof. dr. Igor BELIČ[†], 19. 12. 1986
- Dr. Marta BLINC[†], 19. 12. 1986
- Prof. dr. Bojan DRŽAJ[†], 19. 12. 1986
- Dr. Jože FEGEŠ[†], 19. 12. 1986
- Prof. dr. Vera JOHANIDES[†], 19. 12. 1986
- Prof. dr. Roman MODIČ[†], 19. 12. 1986
- Prof. dr. Tihomir NOVAKOV, 19. 12. 1986
- Prof. dr. Robert LAFFERTY, 15. 6. 1994
- Prof. dr. Walter STEINER, 15. 6. 1994
- Prof. dr. D. Luc MASSART[†], 8. 3. 1995
- Prof. dr. John R. HELLIWELL, 21. 10. 1996
- Prof. dr. Joachim MAIER, 17. 4. 1996
- Prof. dr. Dušan HADŽI, 9. 10. 2001

Finance

PRIHODKI (1000 SIT)

	2006	2005	Struktura 2006 (%)	Indeks 2006/2005
Raziskovalni programi	869.870	856.648	31	102
Infrastrukturni programi	100.356	97.950	3	102
Raziskovalni projekti	270.742	289.270	10	94
Ustanoviteljske obveznosti	359.764	408.295	13	102
Mladi raziskovalci	306.270	241.720	11	127
Domači trg	511.591	454.089	18	113
Tuji trg	160.588	125.495	6	128
Drugi prihodki	225.193	115.206	8	132
SKUPAJ PRIHODKI	2.804.374	2.588.673	100	108

ODHODKI (1000 SIT)

	2006	2005	Struktura 2006 (%)	Indeks 2006/2005
Stroški materiala	-325.226	-278.473	12	117
Stroški storitev	-403.942	-356.006	15	113
Amortizacija	-261.169	-249.974	10	104
Stroški dela	-1.642.774	-1.512.741	61	109
Drugi odhodki	-40.805	-30.890	2	132
SKUPAJ ODHODKI	-2.673.916	-2.428.084	100	110

REZULTAT POSLOVANJA	130.458	160.589	-	81
----------------------------	----------------	----------------	----------	-----------

Finances

REVENUES (1000 SIT)

	2006	2005	Structure 2006 (%)	Index 2006/2005
Research programmes	869.870	856.648	31	102
Infrastructure programmes	100.356	97.950	3	102
Research projects	270.742	289.270	10	94
Overhead financing	359.764	408.295	13	102
Young researchers	306.270	241.720	11	127
Domestic market	511.591	454.089	18	113
Foreign market	160.588	125.495	6	128
Other incomes	225.193	115.206	8	132
TOTAL	2.804.374	2.588.673	100	108

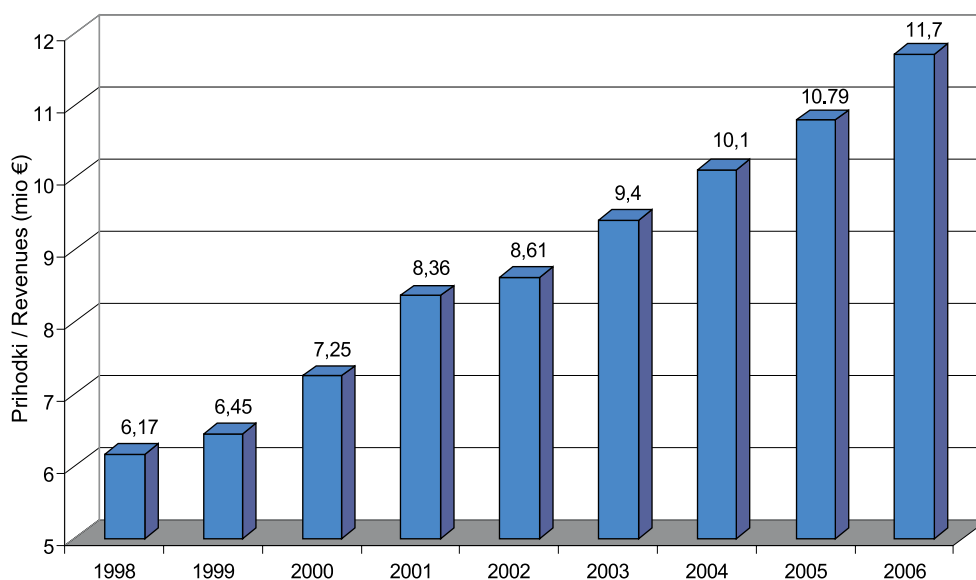
OUTFLOW (1000 SIT)

	2006	2005	Structure 2006 (%)	Index 2006/2005
Costs of material	-325.226	-247.922	12	117
Costs of services	-403.942	-317.147	15	113
Depreciation	-261.169	-230.183	10	104
Labour costs	-1.642.774	-1.459.714	61	109
Other outcomes	-40.805	-61.953	2	132
TOTAL	-2.673.916	-2.316.919	100	110

FINAL RESULT	130.458	160.589	-	81
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Prihodki Kemijskega inštituta

Revenues of the National Institute of Chemistry



SLIKA

Prihodki Kemijskega inštituta v mio EUR.

FIGURE

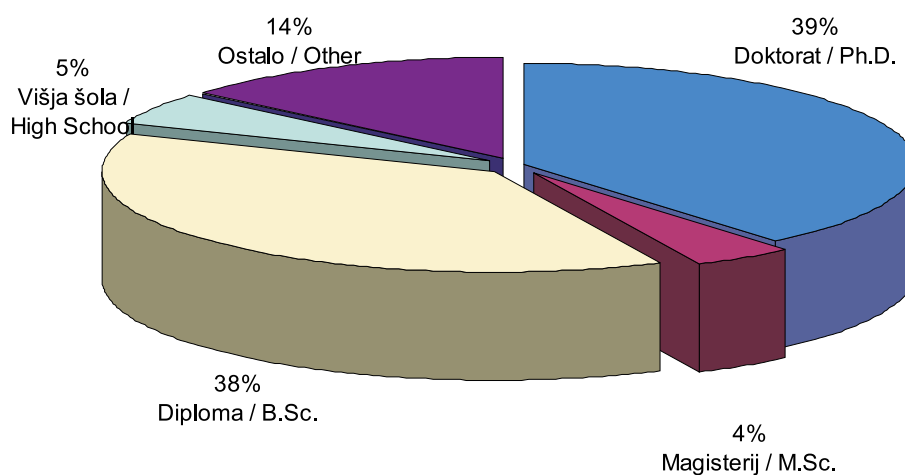
Revenues of the National Institute of Chemistry in million euros.

Zaposleni

Personnel

Na dan 31. 12. 2006 je bilo na Kemijskem inštitutu 241 zaposlenih, od tega 95 doktorjev znanosti, 9 magistrov, 91 z visoko izobrazbo, 12 z višjo izobrazbo, 24 s srednjo in 10 z nižjo izobrazbo. Število zaposlenih se je glede na predhodno leto povečalo za 6 %, predvsem na račun uspešnih prijav na razpis za mlade raziskovalce.

On December 31, 2006, we have recorded 241 employees with the following degree of education: Ph.D. (95), Master degree (9), Bachelor degree (91), Associate degree (12), secondary school (24) and less than secondary school (10). Compared to the previous year the number of employees rose by 6 %, mainly due to a number of successful applications for the "Young Researcher" tender.



SLIKA
Izobrazbena struktura zaposlenih na Kemijskem inštitutu v letu 2006.

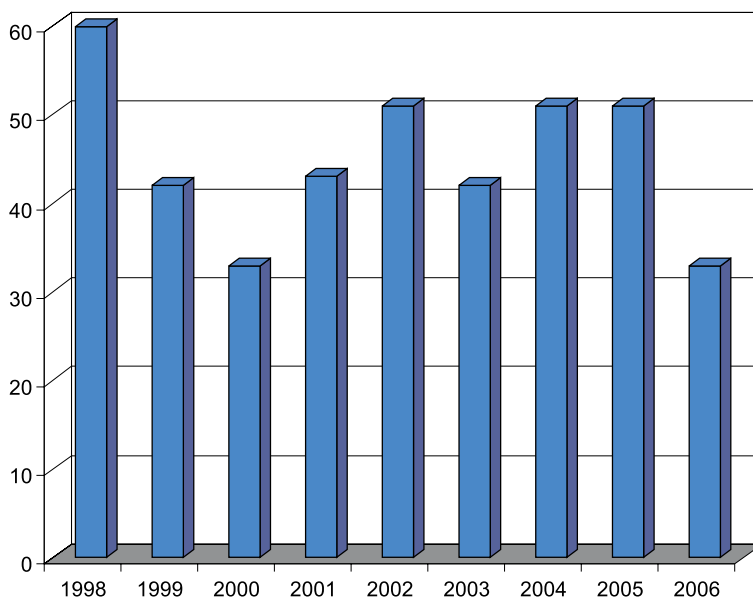
FIGURE
Employees level of education at the National Institute of Chemistry in 2006.

Doktorati, magisteriji in diplome v letu 2006

Doctoral, Master's and Graduate Theses in Year 2006

DOKTORATI / DOCTORAL THESES

- Mojca Fir, 11. 12. 2006
- Robi Ješe, 8. 3. 2006
- Mateja Novak Štagoj, 24. 10. 2006



SLIKA
Doktorati, magisteriji in diplome v letih
1998 / 2006.

FIGURE
Ph.D., M.Sc., and B.Sc. theses in years
1998 / 2006.

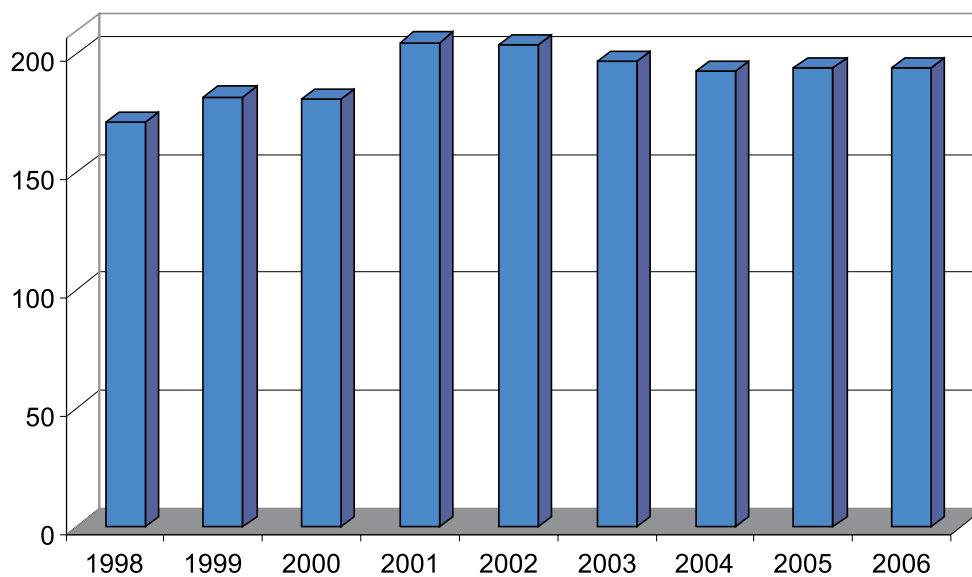
**ŠTEVILO DIPLOM, MAGISTERIJEV, DOKTORATOV, MENTORSTEV IN KOMENTORSTEV S
STRANI ZAPOSLENIH NA KEMIJSKEM INŠTITUTU**

**NUMBER OF B. Sc., M. Sc., Ph. D. THESES, MENTORSHIPS AND COMENTORSHIPS BY
EMPLOYEES OF NATIONAL INSTITUTE OF CHEMISTRY**

1	diploma / Undergraduate Thesis
1	magisterij / Master's Thesis
3	doktorati / Doctoral Theses
6	mentorstev pri diplomah / Mentorships of Undergraduate Theses
4	mentorstva pri magisterijih / Mentorships of Master's Theses
2	mentorstvi pri doktoratih / Mentorships of Doctoral Theses
16	komentorstev pri diplomah / Comentorships of Undergraduate Theses
2	komentorstvi pri magisterijih / Comentorships of Master's Theses
14	komentorstev pri doktoratih / Comentorships of Doctoral Theses

Objave v letu 2006

Published Works in Year 2006



SLIKA
Objavljena dela (članki, knjige, poglavja, patenti) v letih 1998 / 2006.

FIGURE
Published works (papers, books, chapters, patents) in years 1998 / 2006.

Bibliografija inštituta v letu 2006
ANALITIČNI PODATKI (tipologija COBISS /
laboratoriji)

Institute bibliography for 2006
ANALYTICAL DATA (typology COBISS /
laboratories)

Dela / Works	L01	L02	L03	L04	L05	L06+ CVTA	L07	L08	L09	L10	L11	L12	L13	L14	NMR	Bruto	Dvojniki/ Overlaps	SKUPAJ / ALL
Članki, monografije, poglavja / Articles, monographies, chapters	43	21	25	12	6	7	15	3	15	17	28	12	7	5	4	220	2	218
Prispevki na konferencah / Conference contributions	37	32	21	23	33	19	33	0	10	25	13	18	7	10	20	301	19	282
Patenti / Patents	0	1	0	0	0	2	5	5	0	0	2	3	1	0	0	19	1	18
Predavanja / Lectures	19	1	4	2	10	0	2	0	3	2	5	11	3	0	4	66	0	66
Dokumenti / Documents	0	3	0	8	14	0	1	0	0	1	0	1	2	11	0	41	0	41
Doktorati, magisteriji, diplome / PhD, MSc, BSc	1	4	0	1	6	3	3	0	0	1	8	3	1	2	0	33	0	33
SKUPAJ / ALL UNITS	100	62	50	46	69	31	59	8	28	46	56	48	21	28	28	680	22	658

Mednarodno sodelovanje

International Cooperation

MULTILATERALNO SODELOVANJE / MULTILATERAL COOPERATION	
5. Okvirni program EU / 5th Framework Programme EU	1
6. Okvirni program EU / 6th Framework Programme EU	14
COST	5
PROTEUS	3
Skupno / Total	23

BILATERALNO SODELOVANJE / BILATERAL COOPERATION	
Argentina / Argentine	1
Češka / Czech Republic	1
Francija / France	3
Hrvaška / Croatia	7
Italija / Italy	1
Indija / India	4
Japonska / Japan	1
Kitajska / China	1
Madžarska / Hungary	1
Makedonija / Macedonia	2
Romunija / Romania	1
Srbija in Črna gora / Serbia and Montenegro	2
Turčija / Turkey	1
Velika Britanija / Great Britain	2
ZDA / USA	7
Skupno / Total	35

Nagrade podeljene sodelavcem inštituta v letu 2006

Awards Given To Collaborators with the Institute in 2006

Ob 60. letnici Kemijskega inštituta so bile prvič podeljene prestižne Preglove nagrade (Grand Hotel Union, Ljubljana, 29. maj 2007)

Veliko Preglovo nagrado Kemijskega inštituta za raziskovalno delo je prejel akademik prof. dr. Dušan Hadži, za izjemne znanstvene dosežke na različnih raziskovalnih področjih.

The prestigious Pregl Awards were awarded for the first time at the occasion of the 60th anniversary of the National Institute of Chemistry (Grand Hotel Union, Ljubljana, May 29, 2007)

The Grand Pregl Award of the National Institute of Chemistry for Research Work was awarded to Member of the Slovenian Academy of Sciences Professor Dušan Hadži for his outstanding work in various fields of research.



Direktor, doc. dr. Peter Venturini izroča Veliko Preglovo nagrado akademiku, prof. Dušanu Hadžiju

The Director of NIC, Dr. Peter Venturini, awards the Grand Pregl Award to Member of the Slovenian Academy of Sciences Professor Dušan Hadži

Preglovo nagrado Kemijskega inštituta za izjemne dosežke je prejel prof. dr. Janez Plavec, za pomembne znanstvene dosežke na področju raziskav gradnikov nukleinskih kislin z uporabo magnetne resonance.

Preglova nagrada Kemijskega inštituta za izjemno doktorsko delo na področju kemije in sorodnih ved, 24. 4. 2007:

- **dr. Primož Šket**: NMR študije vezave kovinskih ionov znotraj G-kvadrupleksnih struktur DNK; mentor: doc. dr. Janez Plavec

Tekmovanje iGEM (international Genetically Engineered Machines), na univerzi Massachusetts Institute of Technology (MIT), Cambridge, ZDA; 5. 11. 2006

Na mednarodnem tekmovanju študentskih ekip iz sintezne biologije je zmagala slovenska ekipa, ki je raziskovalno delo opravljala na Kemijskem inštitutu ter na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani. Ekipo sta vodila prof. dr. Roman Jerala s Kemijskega inštituta in doc. dr. Marko Dolinar s Fakultete za kemijo in

The Pregl Award of the National Institute of Chemistry for outstanding achievements was received by Professor Janez Plavec, for his important scientific achievements in the research of nucleic acid building blocks using magnetic resonance.

The Pregl Award of the National Institute of Chemistry for outstanding doctoral work in the field of chemistry and related sciences, April 24, 2007:

- **Dr. Primož Šket**: NMR Studies of cation binding within G-quadruplex DNA structures; mentor: Dr. Janez Plavec, Assist. Prof.

iGEM (international Genetically Engineered Machines) Competition, Massachusetts Institute of Technology (MIT), Cambridge, USA, Nov. 5, 2006

At an international competition of student teams in the field of synthetic biology, the Slovenian team, which had carried out its research at the NIC and the Faculty for Chemistry and Chemical Technology of the University of



Prof. Janezu Plavcu je med prvimi čestital premier Janez Janša

Prof. Janez Plavec was among the first to be congratulated by Prime Minister Janez Janša

kemijsko tehnologijo Univerze v Ljubljani, študenti pa so bili z Biotehniške fakultete (študij mikrobiologije), Fakultete za matematiko in fiziko ter Fakultete za kemijo in kemijsko tehnologijo (vse Univerza v Ljubljani). Pri izvedbi projekta so kot mentorji sodelovali tudi raziskovalci Laboratorija za biotehnologijo Kemijskega inštituta.

Heureka! 06 - osrednja slovenska prireditev na področju inovativnosti (24.-27. oktober 2006, Ljubljana).

- Raziskovalna skupina Laboratorija za biotehnologijo pod vodstvom prof. dr. Romana Jerale je bila uvrščena med 17 najboljših raziskovalnih skupin v letu 2005.

Ljubljana, won. The team was lead by Dr. Roman Jerala from the NIC and Dr. Marko Dolinar from the Faculty for Chemistry and Chemical Technology of the University of Ljubljana, while the students were from the Biotechnical Faculty (studying microbiology) and the Faculty of Mathematics and Physics at the University of Ljubljana. Researchers from the Laboratory for Biotechnology of the NIC worked as mentors on the project.

Heureka! 06 – central Slovenian event in the field of innovation (October 24-27, 2006, Ljubljana)

- Research group from the Laboratory for Biotechnology under the leadership of Prof.



Dr. Primož Šket

Inovacija »Nova vodotopna oblika koencima Q10, njegova priprava in uporaba«

je prejela dve priznanji:

- **Zlato priznanje Gospodarske zbornice Slovenije - Območne zbornice Ljubljana**, 23. 05. 2006 in
- **Zlato priznanje Gospodarske zbornice Slovenije**, 28. 06. 2006

Avtorji inovacije so raziskovalci Kemijskega inštituta: dr. Mirko Prošek, dr. Janko Žmitek, dr. Andrej Šmidovnik, dr. Alenka Golc Wondra, dr. Samo Andrenšek, Maja Fir in dr. Monika Stražičar.

Kemijski inštitut je ob mestnem prazniku, dveh miru, prejel nagrado glavnega mesta Ljubljana, 09. 05. 2006

36. Krkine nagrade 2006; Novo mesto, 27. 10. 2006

- **Dr. Primož Šket**: »NMR študije vezave kovinskih ionov znotraj G-kvadrupleksnih struktur DNK«; mentor: doc. dr. Janez Plavec

Roman Jerala was among the 17 best research groups in 2005.

Innovation "New water soluble form of Coenzyme Q10, its preparation and use"

received two awards:

- **Gold Award, Chamber of Commerce of Slovenia – Regional Chambers Ljubljana**, May 23, 2006 and
- **Gold Award, Chamber of Commerce of Slovenia**, June 28, 2006

Authors of innovation were researchers from the NIC: Dr. Mirko Prošek, Dr. Janko Žmitek, Dr. Andrej Šmidovnik, Dr. Alenka Golc Wondra, Dr. Samo Andrenšek, Maja Fir and Dr. Monika Stražičar.

At the occasions of the Day of Peace the NIC received the award of the capital city, Ljubljana, May 9, 2006

36th Annual Krka Prizes, Novo mesto, Slovenia; October 27, 2006:

- **Dr. Primož Šket**: »NMR Studies of cation



Zmagovalna ekipa študentov Ljubljanske univerze na sprejemu pri direktorju Kemijskega inštituta (iGEM, 2006)

The winning team of students from the University of Ljubljana with the Director of NIC (iGEM, 2006)



Dr. Franci Demšar, direktor ARRS izroča priznanje prof. dr. Romanu Jerali (Hevrek! 06)

Dr. Franci Demšar, director of ARRS (Slovenian Research Agency) handing Prof. Roman Jerala the award (Heureka! 06)



Zlati priznanji Gospodarske zbornice Slovenije



Gold Awards, Chamber of Commerce of Slovenia

- **Aljaž Godec:** »Vpliv prostorske restrikcije na nastanek in stabilnost polimorfnih oblik«; mentor: doc. dr. Miran Gaberšček
- **Uroš Maver:** »Stresalna naprava z modificiranimi polimernimi siti za ločevanje in analizo velikosti delcev«; mentor: dr. Marjan Bele
- **Borut Zupančič:** »Novi katalizatorji za asimetrično hidrogeniranje«; mentorja: dr. Michael Stephan, dr. Barbara Mohar

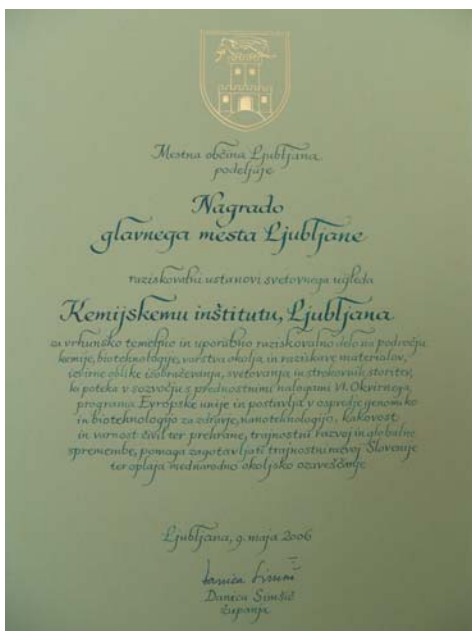
Prešernove nagrade študentom Fakultete za kemijo in kemijsko tehnologijo, Univerza v Ljubljani, 8. 12. 2006

- **Andrej Žnidaršič:** »Sinteza prahov in prevlek na osnovi kalcijevih fosfatov za uporabo v medicini in farmaciji«; mentor: doc. dr. Miran Gaberšček, somentor: dr. Marjan Bele

- binding within G-quadruplex DNA structures«; mentor: Dr. Janez Plavec, Assist. Prof.
- **Aljaž Godec:** »The influence of space restriction on the formation and stability of polymorphs«; mentor: Dr. Miran Gaberšček, Assist. Prof.
- **Uroš Maver:** »New sieving device with modified polymeric sieves for separation and particle size analysis«; mentor: Dr. Marjan Bele
- **Borut Zupančič:** »New Catalysts for Asymmetric Hydrogenation«; mentors: Dr. Michael Stephan, Dr. Barbara Mohar

Faculty Prešeren Prize presented by the Faculty of Chemistry and Chemical Technology of the University of Ljubljana, Slovenia for Undergraduate Thesis Work; December 8, 2006:

- Andrej Žnidaršič:** »Synthesis of powders and coatings based on calcium phosphates for application in medicine and pharmaceuticals«; mentor: Dr. Miran Gaberšček, Assist. Prof., comentor: Dr. Marjan Bele



Nagrada glavnega mesta Ljubljana



The Award of the capital city, Ljubljana

Zaposleni v splošnem sektorju

General Sector - Employees



UPRAVA / ADMINISTRATION

Izidor Babnik
Francka Dobnikar
Muharem Husić
Saša Lah
Marija Merzel
Vida Petrovčič
Brigita Pirc
Jadranka Požanel
Tanja Svetic
Velesa Tovšak
Andreja Zupančič

TEHNIČNE DELAVNICE / TECHNICAL SERVICES

Vladimir Mrzel (vodja / head)
Toni Ambrož
Gregor Babnik
Marjan Smole
Robert Vidmar
Pavle Vrhovec

RAČUNOVODSTVO, PLAN IN ANALIZE / ACCOUNTING, PLANNING AND ANALYSES

Barbara Dorić
Vedrana Gorenšek
Maja Mirić
Janja Pintarič
Irena Oblak
Zlatka Skok
Radovan Stritih
Tanja Volovšek

KNJIŽNICA / LIBRARY

Lilijana Grah
Lucija Kramberger
Zdenka Laznik

ŠTIPENDIJE / SCOLARSHIPS

Alen Kljajič
David Šarlah
Peter Miklavc

L01

Laboratorij za molekularno modeliranje in NMR spektroskopijo

Laboratory for Molecular Modelling and NMR Spectroscopy



VODJA / HEAD
prof. dr. Branko Borštnik

RAZISKOVALCI / RESEARCHERS

dr. Franc Avbelj
dr. Simona Golič Grdadolnik
dr. Jože Grdadolnik
dr. Milan Hodošček
dr. Dušanka Janežič
doc. dr. Janez Mavri
dr. Franci Merzel
dr. Ksenija Poljanec
dr. Matej Praprotnik
dr. Danilo Pumpernik
dr. Jernej Stare
prof. dr. Tomaž Šolmajer
dr. Gregor Mlinšek
mag. Dragan Lukman
Špela Klofutar

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Urban Borštnik
Urban Bren
Nejc Carl
Janez Konc
Borut Tone Oblak
Mihael Simčič
Tjaša Urbič
Jernej Zidar

TEHNIČNO OSEBJE / TECHNICAL STAFF

Tatjana Karba
Silva Zagorc



PODROČJA DEJAVNOSTI

Raziskovalni program P1-0010 (F. Avbelj)

Folding in dinamika biomolekularnih sistemov

- Raziskave strukture in dinamike biomolekularnih sistemov (proteinov, ligandov, membran in njihovih kompleksov) z jedrsko magnetno resonanco, vibracijsko spektroskopijo in z računalniškimi simulacijami (Monte Carlo, molekulska dinamika);
- študij elektrostatskih interakcij, vodikovih vezi, solvatacije (elektrostatsko senčenje) in hidrofobnih interakcij v proteinih, v sistemih ligand-receptor in v sistemih biomolekula-membrana;
- študij energetike in kinetike zvitja proteinov;
- razvoj algoritmov za napovedovanje sekundarnih in tridimenzionalnih struktur proteinov (problem zvitja proteinov »protein folding problem«, strukturna genomika);
- konformacijske študije novih učinkovin v povezavi z njihovim biološkim učinkom;
- razvoj metod vibracijske spektroskopije (računanje optičnih konstant iz refleksijskih in ATR spektrov);

RESEARCH ACTIVITIES

Research program P1-0010 (F. Avbelj)

Protein Folding and Dynamics of Biomolecular Systems

- Studies of structure and dynamics of biomolecular systems (proteins, ligands, membranes, and related complexes) using nuclear magnetic resonance, vibrational spectroscopy, and computer simulations (Monte Carlo, molecular dynamics)
- Studies of electrostatic interactions, hydrogen bonds, solvation (electrostatic screening), and hydrophobic interactions in proteins, ligand-receptor and ligand-membrane complexes
- Studies of energetics and kinetics of the protein folding process
- Development of algorithms for predicting secondary and three-dimensional structure of proteins (protein folding problem, structural genomics)
- Conformational studies of novel drugs in relation with their biological activity
- Development of new methods for vibration-

- študij vodikovih vezi z eksperimentalnimi in teoretskimi metodami;
- razvoj metod jedrske magnetne resonance za določanje konformacije molekul v tekočini;
- uporaba vibracijske spektroskopije in jedrske magnetne resonance v analizne namene.

Raziskovalni program P1-0012 (B. Borštnik)
Molekulske simulacije in bioinformatika

- Kvantno kemijski izračuni strukturnih in elektronskih parametrov molekul in supramolekularnih sistemov;
- študij dinamike tvorbe in razpada medmolekularnih vezi in dinamike reakcij prenosa atoma (atom-transfer reactions);
- simulacija prenosa protona v hidratiranih sistemih z metodami klasične in kvantne molekularne dinamike;
- študij endogene karcinogeneze;
- bioinformatika in študij biološke evolucije na molekularni osnovi;
- statistična mehanika;
- racionalno načrtovanje novih zdravilnih učinkovin na osnovi strukture receptorja in proučevanja mehanizma inhibicije encimov.

Raziskovalni program P1-0002 (D. Janežič)
Računalniško modeliranje strukture in dinamike molekul

Raziskovalna projekta:

J1-6331: (D. Janežič)

Razvoj računalniških algoritmov za simulacije makromolekularnih sistemov

J1-5115: (F. Merzel)

Simulacije in strukturna analiza vode ob površini proteinov

Razvoj in uporaba metod za molekularno modeliranje:

- simplektične metode za simulacijo molekulske dinamike makromolekul;
- kombinacije metod simulacije molekulske dinamike, analize po normalnih načinih nihanja in kvaziharmonske analize proteinov v raztopinah za študij hidratacije proteinov;
- razvoj in uporaba QM/MM metod;

al spectroscopy (calculation of optical constants)

- Studies of hydrogen bonding using experimental and theoretical methods
- Development of new methods for conformational studies of molecules by the high-resolution nuclear magnetic resonance spectroscopy
- Application of nuclear magnetic resonance spectroscopy and vibrational spectroscopy in chemical analysis

Research program P1-0012 (B. Borštnik)
Molecular Simulations and Bioinformatics

- Quantum chemical calculations of structural and electronic parameters of molecules and supramolecular systems.
- Studies of dynamics of formation and decay of intermolecular bonds atom-transfer reactions
- Simulation of proton transfer reactions in hydrated systems using the methods of classical and quantum molecular simulations
- Study of endogeneous cancerogenesis
- Bioinformatics and the study of biological evolution
- Statistical mechanics
- Structure-based drug design approach is used for mechanistic studies of enzyme inhibition and design of novel bioactive compounds

Research program P1-0002: (D. Janežič)
Computer Simulation of Molecular Structure and Dynamics

Research projects:

J1-6331: (D. Janežič)

Computer Algorithms Development for Macromolecular Simulation

Development and application of methods for molecular modeling:

- Symplectic methods for molecular dynamics simulations of macromolecules
- Combination of molecular dynamics methods, normal mode vibrational analysis, and quasiharmonic analysis of proteins in solutions for studying protein hydration

- razvoj računsko učinkovitih metod za določanje časovno odvisne elektronske strukture molekul na osnovi Kohn-Sham-ove formulacije teorije gostotnih funkcionalov;
- razvoj in aplikacija kvantno kemijskih in klasičnih pristopov za izračun reakcijskih mehanizmov, predvsem za izračun ionskih reakcij izocianidov;
- razvoj in uporaba formalizma RISM;
- razvoj novih in učinkovitih računalniških topologij za povezovanje osebnih računalnikov v računalniške gruč.

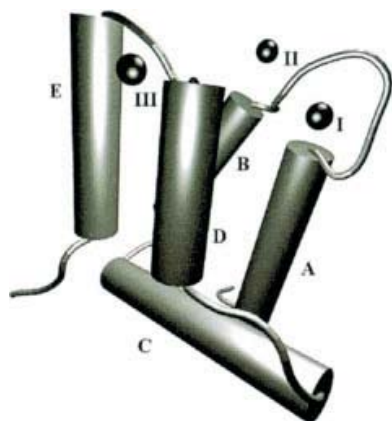
BIBLIOGRAFIJA

- 38 izvirnih znanstvenih člankov
- 1 samostojni znanstveni sestavek v monografiji
- 1 intervju
- 3 drugi članki ali sestavki
- 4 objavljeni znanstveni prispevki na konferencah

- Development and use of QM/MM methods
- Development of computationally efficient methods for determining the time-dependent electronic structure of molecules based on the Kohn-Sham formulation of the density functional theory
- Development and application of quantum chemical and classical approaches for calculating reaction mechanisms, especially calculating the ionic reactions of isocyanides
- Development and use of the RISM formalism
- Development of new and effective network topologies for connecting personal computers into computational clusters

BIBLIOGRAPHY

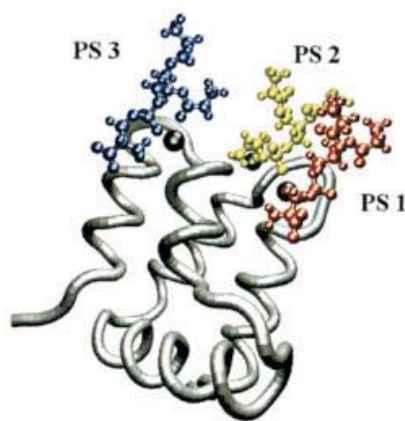
- 38 Original Scientific Articles
- 1 Independent Scientific Component Part in a Monograph
- 1 Interview
- 3 Other Articles or Component Parts



(a) ANX V/1

SLIKA 1:

(a) Sekundarna struktura domene 1 aneksina V (ANX V/1). Oznake od A do E označujejo karakteristike vijačnic. Črne kroglice I-III kažejo lege treh kalcijevih ionov. (b) Vezava aneksina z membrano: tri fosfatidilserinske molekule v kompleksu z ANX V/1 povezane s tremi kalcijevimi ioni.



(b) ANX V/1 + PS

FIGURE 1:

(a) Secondary Structure of Annexin V, domain 1 (ANX V/1). Labels A to E denote the characteristic helices. Black spheres I-III show the position of three calcium ions. (b) Prototype of an annexin-membrane binding: three phosphatidylserine (PS) molecules in complex with ANX V/1 involving three calcium ions.

31	objavljenih povzetkov znanstvenih prispevkov na konferencah	4	Published Scientific Conference Contributions
2	objavljena povzetka strokovnih prispevkov na konferencah	31	Published Scientific Conference Contribution Abstracts
10	predavanj na tujih univerzah	2	Published Professional Conference Contribution Abstracts
4	prispevki na konferencah brez natisa	10	Invited Lectures at Foreign Universities
5	vabljenih predavanj na konferencah brez natisa	4	Unpublished Conference Contributions
1	diploma	5	Unpublished Invited Conference Lectures
4	uredništva revij	1	Undergraduate Thesis
		4	Journal Editorships

GLAVNI DOSEŽKI V LETU 2006

Agregacija prionskih proteinov v fibrile povzroča bolezni, kot so: BSE, diabetes tipa II, Alzheimerjevo in Parkinsonovo bolezen. Fizikalni razlog za tvorbo fibrilov ni poznan. Postavili smo hipotezo, da β -trakovi v denaturiranem stanju tvorijo nukleacijska mesta za nespecifično vezavo v večje β -plasti (β -sheet) s pomočjo meh-anizma zadrge. Hipoteza temelji na našem odkritju, da nekateri predeli proteinov tvorijo iztegnjene β -trakove (β -strand) že v denaturiranem stanju. Hipotezo smo potrdili na mutantih stefina. Pokazali smo, da obstaja korelacija med tendenco tvorbe fibrilov in tendenco tvorbe β -trakov v denaturiranih proteinih.

Derivati piridiletanol(fenetil)aminov imajo visoko afiniteto do različnih receptorjev. Najpomembnejši primer je inhibicija biosinteze holesterola. Z uporabo NMR metod smo identificirali in razložili mehanizem dinamičnega procesa, ki je posledica inverzije centralnega aminskega dušika in povzroča zanimiv primer diasteromernega efekta pri tej vrsti spojin. Z analizo jedrskega Overhauser-jevega efekta (NOE) in molekularno orbitalnimi izračuni smo določili konformacijske lastnosti diasteromernega para. Študirali smo konformacijske zahteve za biološko aktivnost linearnih peptidnih antagonistov mielinskega proteina, ki inhibirajo modelni eksperimentalni sistem EAE za študij skleroze multipleks. Z metodami NMR spektroskopije in molekularnega modeliranja smo identificirali posamezne populacije antagonistov v raztopini, ki so v skladu z NOE kontakti, in jih primerjali s kristalno strukturo nativnega agon-

IMPORTANT ACHIEVEMENTS IN 2006

The aggregation of amyloid-forming proteins (prions) in fibrils is characteristic of human neurodegenerative diseases, including transmissible spongiform encephalitis, type II diabetes, Alzheimer's and Parkinson's diseases. The physical background of fibril nucleation is unclear. We presumed that the aggregation into fibrils is caused by fluctuating β -strands in denatured proteins. These local structures present a nucleus in the denatured state that seeds the non-specific assembly of other parts of a polypeptide chain into a large β -sheet structure, presumably by a zipper mechanism. We found relatively good correlation of the fibrillisation propensity of stefin mutants with the propensity of forming β -strands in the specific regions of a protein.

Derivatives of pyridylethanol (phenethyl)-amines display high affinities for various receptors; a notable example is the inhibition of cholesterol biosynthesis in a cell assay. By application of NMR methods we identified and explained the mechanism of a dynamic process due to nitrogen inversion at the central amine nitrogen, which is causing an interesting case of the diastereomeric effect in these compounds. The conformational properties of the diastereomeric pair were determined by the analysis of NOE connectivities and MO calculations.

Conformational requirements for antagonist activity of linear peptide ligands of myelin basic protein were investigated by NMR and molecular modeling methods. These linear pep-

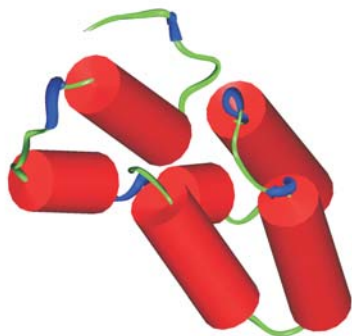
ista v trimolekularnem kompleksu s HLA-DR2b in T-celičnim receptorjem (TCR). Ugotovili smo, da imajo antagonisti drugačno topologijo aminokislinskega ostanka Phe⁹⁸, kot jo ima nativni agonist. Phe⁹⁸ agonista je v kontaktu s TCR. Zato predpostavljamo, da je razlog za antagonistično delovanje raziskanih linearnih peptidov izguba hidrofobne interakcije stranske verige fenilalanila s TCR, kar preprečuje aktivacijo T-celic.

Z infrardečo spektroskopijo smo raziskovali termodinamske lastnosti monoalkilnih fenolnih lipidov z dvema različnima polarnima glavama (fenol, N-piperidin metil fenol). Pokazali smo, da se v fenolnih lipidih tvori srednje močna intermolekularna vodikova vez. Nasprotno pa je glavna značilnost lipidov z N-piperidin metil fenol polarno glavo tvorba močne intramolekularne vodikove vezi med fenolno skupino in dušikom iz piperidinskega obroča. Intramolekularna vodikova vez preprečuje hidratacijo in določa temperaturo glavnega faznega prehoda. V lipidnih dvoslojih s diacil fosfolipidom se intramolekularna vodikova vez v N-piperidin metil fenolu ohrani, medtem ko fenolna OH skupina močno veže s fosfatno skupino. Lipidni dvosloj z diacil fosfolipidi pa v obeh primerih zniža temperaturo faznega prehoda.

Pri študiju vpliva nizkih temperatur na kratke vodikove vezi med karboksilno skupino vezane kisline in hidratno vodo v kristalnem dihidratu smo opazili v infrardečih in ramanskih spektrih

tides were found to inhibit experimental autoimmune encephalomyelitis, which is a model system of multiple sclerosis. Distinct populations of antagonist, which are in agreement with NOE data, were identified and compared with the X-ray structure of native agonist in a tri-molecular complex with a Human Leukocyte Antigen (HLA-DR2b) and T-cell receptor (TCR). In antagonist different topology of residue Phe⁹⁸ with respect to native agonist was found. The Phe⁹⁸ of the agonist is in a contact with TCR. It is proposed that the antagonistic activity of investigated peptides may be due to the loss of some hydrophobic interactions between the phenyl side chain and TCR, which hinders the activation of T-cells.

The thermodynamic properties of 3-pentadecylphenol (PDP) and 3-pentadecyl 2-(N-piperidine methyl) phenol (PPMP) were investigated using vibrational spectroscopy. The PDP lipid forms a medium strong intermolecular H-bond. The PPMP lipid forms a stronger intramolecular H-bond with broad OH stretching. Both types of H-bonds prevent the hydration of lipid films. The differences in H-bonding are also reflected in the diverse temperatures of the main transition (T_m). In mixtures with dialcylphosphatidylcholine lipid (DPPC), both lipids significantly reduce the T_m for DPPC. The OH group of the PDP lipid strongly interacts with the phosphate group from DPPC. For PPMP no



SLIKA 2:

Primerjava med eksperimentalno (leva slika) in napovedano 3D strukturo proteina T097.

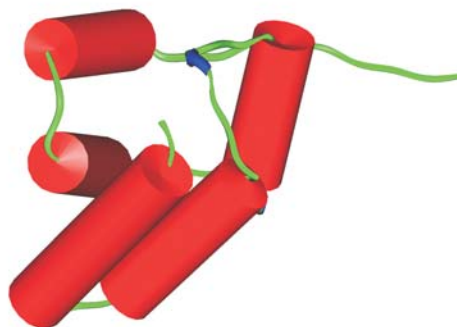


FIGURE 2:

Comparison between x-ray structure (left) and predicted 3D structure of protein T097.

tvorbo hidronijevega iona, kar nas je navedlo na meritve prevodnosti. Meritve pri različnih frekvencah so pokazale na tvorbo polaronov. Ker sproščanje elektronov pri tej snovi ni verjetno, so očitno nosilci naboja hidronijeve ioni. To je po našem vedenju prvi primer tvorbe polaronov s temi ioni.

Preučevali smo kemijsko reakcijo med končnimi karcinogeni in DNA (gvanin na poziciji N7). Kvantno kemijski izračuni skupaj z različnimi solvatacijskimi modeli dajo aktivacijske energije, ki so v skladu z eksperimentom. To so prvi izračuni kemijske reaktivnosti DNA s končnimi karcinogeni epoksidnega tipa.

Preučevali smo dinamiko prenosa protona v vodikovo vezanih sistemih in encimskih centrih. Zanesljive simulacije dinamike protona zahtevajo kvantno dinamsko obravnavo zaradi kvantne narave gibanja jeder. Razvijali smo računsko metodologijo za tovrstne simulacije. Metodologijo smo uporabili za študij vibracijske dinamike vodikovo vezanih sistemov (substituirani N-oksidi pikolinske kisline), ki se odražajo v vibracijskih spektrih. Delo je potekalo v sodelovanju s prof. Hadžijem, ki je vodil eksperimentalni del raziskav. Razvito metodologijo smo uporabili za simulacijo prenosa vodika v encimu lipoksigenaza skupaj z dr. Warshelom.

Delali smo na razvoju metodologije izračunov proste energije v bioloških sistemih in aplikacijah metodologije na DNA polimerazi.

Preučevali smo asimetrijo točkovnih mutacij med približno tridesetimi milijoni sprememb nukleotidov, ki ločijo človeka od šimpanza. Analiza je pokazala, da so tranzicije (zamenjave znotraj razreda purinov oziroma pirimidinov) štirikrat bolj pogoste kot transverzije (zamenjave purinov s pirimidini). Ugotovili smo tudi, da tranzicije bogatijo človeški genom z nukleotidi, ki so v DNA vijačnici povezani s trojno vodikovo vezjo (citozin in gvanin), neto učinek tranzicij pa je ravno nasproten.

V okviru dela na raziskovalnem programu P1-0002 smo v letu 2006 objavili 14 originalnih znanstvenih člankov, od tega 10 v SCI revijah, od katerih jih je 6 v SCI revijah iz prvega kvarti-

such interaction can be observed. Mixing of PPMP with various amounts of DPPC preserves the intra-molecular H-bond between the piperidinic nitrogen and the OH group, which is characteristic of pure PPMP films.

Formation of hydroxonium ions was observed in the low temperature infrared and Raman spectra of oxalic acid dihydrate crystals. This led us to investigate the conductivity of the crystals. The results show that polarons are formed at temperatures below 150 K. Since electrons as charge carriers are highly unlikely, the only possible ones may be the hydroxonium ions. To our knowledge, this is the first example of polaron formation with the hydroxonium ion as charge carrier.

We studied chemical reactions between various ultimate carcinogens and DNA (Guanine at position N7). Quantum chemical calculations in conjunction with different solvation models yield activation free energies that are in good agreement with the experiment.

These are the first reported calculations of DNA chemical reactivity with the ultimate carcinogens from the first principles.

We studied dynamics of proton transfer process in hydrogen bonded systems and enzyme centers. Proper description of proton dynamics requires quantum dynamical treatment because of the quantum nature of nuclear motion. We worked on the development of the computational methodology. Applications include vibrational dynamics of strong intramolecular hydrogen bonded systems (substituted picolinic acid N-oxides) reflected in vibrational spectra. This work was performed in collaboration with Dr. Hadži who studied the systems experimentally. The other application of the methodology is for the dynamics of proton transfer in enzyme lipoxygenase, and this study was performed together with Dr. Warshel.

We further developed methodology for calculations of free energy differences that are essential for studies of binding and reactivity and applied it to DNA polymerase.

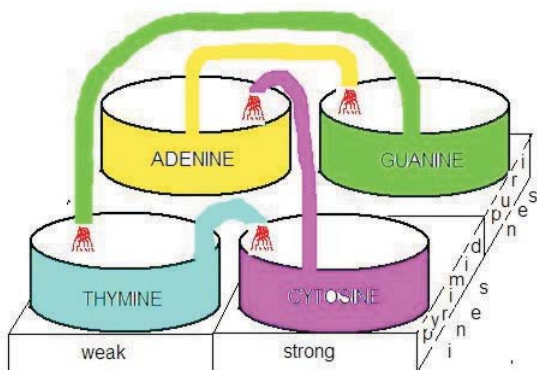
la. Nekateri glavni dosežki so naslednji. Za potrebe relevantnih simulacij aneksina, ki se veže na membrano preko kalcijevih ionov, smo razvili nove parametre za potencialno polje, ki opisuje interakcijo kalcijevih ionov z okolico. S pomočjo kvantno kemijskih računov smo določili potencialne ploskve za kalcijeve ione v treh različnih vezavnih mestih, ki so značilni za domeno 1 aneksina V (ANX V/1). Na podlagi teh izračunov smo določili strukturo vezavnih mest, kvantificirali polarizacijo naboja na atomih v vezavnem mestu ter določili konstante sil za harmonsko sklopitev med Ca ioni ter bližnjimi kisikovimi atomi, ki smo jo vpeljali, da bi minimizirali razliko med klasičnim in kvantnim potencialnim poljem. Pokazali smo, da je z uporabo modificiranega potencialnega polja za kalcijeva vezavna mesta mogoče izvajati MD simulacije na veliki časovni skali, ki ohranjajo strukturne elemente aneksina, kar je neobhodno potrebno za študij delovanja tega proteina. Razvili smo nov algoritem za izračun topilu dostopne molekulske površine (MS) in grafični računalniški program za gibanje po molekulski

The asymmetry of point mutations, which occurred in primate lineage since the last common ancestor to human and chimpanzee, was studied. It was found that transitions (the interchanges within purines or within pyrimidines) are approximately four times more probable than transversions (the replacements of purines with pyrimidines, or vice-versa).

It was also found that the net effect of transitions contributes to a higher level of nucleotides, which are bound by three hydrogen bonds in DNA (cytosine and guanine), while the transversions have an opposite effect.

As part of the work under the research program P1-0002, we published 14 original scientific articles, 10 of which appear in SCI journals and 6 of which are in the first quartile of SCI journals. Some of the major achievements are the following:

For accurate classical molecular dynamics (MD) simulations of the calcium mediated bound complexes of annexin and membrane we have developed new force-field parameters correctly describing the interaction of the Ca ion with



SLIKA 3:

V zadnjih šestih milijonih let človeške evolucije se je genetski zapis v človeškem genomu spremenil za kakšen odstotek, vsebnost štirih nukleotidov (adenina, citozina, gvanina in timina) pa se je manj spremenila. Slika prikazuje smeri neto izmenjav med štirimi nukleotidi, ki ne bi, če bi bili vsi pretoki enaki, spreminjali sestave genoma.

FIGURE 3:

During the last six million years of human evolution the nucleotide sequences defining the human genome changed by approximately one percent while the composition in terms of four nucleotides (adenine, cytosine, guanine and thymine) witnessed lesser change. The figure shows the directions of net mutational flows between four nucleotides. If all the flows would be equal, the composition of the human genome would not change.

površini. Površino dobimo s kotaljenjem krogle, ki predstavlja molekulo topila, prek atomov opazovane molekule. Z uporabo tako dobljene površine v grafičnem računalniškem programu »MS walk« dosežemo nov pogled na molekule. Prednost »MS walk« pristopa je, da lahko opazujemo votline v molekuli, ki so z drugimi metodami le delno vidne. Naš algoritem, čigar časovna zahtevnost raste linearno s številom atomov v molekuli, je primerljiv s podobnimi obstoječimi algoritmi. MS algoritem in »MS walk« program sta dostopna na spletnem naslovu (http://www.cmm.ki.si/konc/ms_walk).

V sodelovanju z Max-Planck institute for polymer research v Mainzu, Nemčija delamo na razvoju adaptivne hibridne simulacijske sheme (Adaptive Resolution Scheme) za učinkovite hibridne atomsko/mezozkopske simulacije molekulske dinamike. Simulacije molekulske dinamike, kjer obravnavamo celoten sistem na atomski skali, so zaradi velikega števila prostostnih stopenj izredno računsko zahtevne. Eden od možnih pristopov, kako zmanjšati računsko zahtevnost, je opis sistema na mezozkopski skali, kjer skupino atomov združimo v en sam delec. S tem znatno zmanjšamo število prostostnih stopenj v sistemu, vendar hkrati izgubimo vez do opisa specifičnih kemijskih lastnosti sistema, za katerega potrebujemo atomsko resolucijo. Edinstvena lastnost novega pristopa je, da dovoljuje dinamično spreminjanje števila molekulskih prostostnih stopenj. Na ta način lahko spreminjamo med atomsko in mezozkopsko resolucijo opisa sistema med samim potekom simulacije molekulske dinamike. To nam omogoča obravnavo le tolikšnega števila prostostnih stopenj, kot je nujno potrebno za dani sistem. Ta pristop je zato idealen za molekularne sisteme, kjer je atomska resolucija potrebna le v nekaterih delih sistema, medtem ko za preostanek sistema zadostuje mezozkopski opis z nižjo stopnjo podrobnosti. Na ta način lahko obravnavamo dolge krajevne in časovne skale, pri čemer se nam ni treba odpovedati opisu sistema na atomski skali, kjer je to potrebno. Učinkovitost novega pristopa je prikazana na

its environment. We have used quantum chemical calculations to investigate the potential energy surface experienced by the Ca ion within the three different binding sites found in domain 1 of annexin V (ANX V/1). Based on these calculations we were able to quantify the charge polarization of atoms within the binding sites and to determine the geometry and force constants of harmonic restraints between a Ca ion and its coordinating oxygen atoms. Harmonic restraints were introduced to compensate for the deviations between the quantum mechanical potential energy surface and that of the classical force field. Our analysis has shown that using the refined force field for the Ca binding sites enables long-time MD simulations that conserve the initial structure of ANX V/1 significantly better than MD simulations using the standard force field.

We designed a new algorithm to compute a solvent accessible molecular surface (MS) and a graphical computer program for a molecular surface walk. The surface is generated by rolling a spherical probe representing a solvent molecule over the atoms of the investigated molecule. We use this surface representation in a graphical computer program MS walk to achieve a new way of viewing the molecules. The advantage of the MS walk approach is that the molecular cavities, only partially visible by using other methods, can be inspected. Our algorithm's performance is comparable to that of similar existing algorithms and its time consumption grows linearly with the number of atoms. The MS algorithm and the MS walk program can be accessed through the Web (http://www.cmm.ki.si/konc/ms_walk).

In collaboration with the Max Planck Institute for polymer research, Mainz, Germany we are working on the development of a new adaptive resolution technique for efficient particle-based multi-scale molecular dynamics (MD) simulations. The presented approach is tailor-made for molecular systems where atomistic resolution is required only in spatially localized domains whereas a lower mesoscopic level of de-

modelskem sistemu tekočine tetraedričnih molekul, ki predstavlja tipičen sistem mehke snovi, t.j. koloidni sistem, metan itd. Simulacijska škatla je razdeljena na dve območji: eno območje vsebuje le tetraedrične molekule z atomsko resolucijo, drugo pa le enodelčne molekule, ki predstavljajo ustrezen mezoskopski model tetraedrične molekule. Molekule lahko prosto prehajajo med obema območjema, pri čemer se ustrezno spreminja stopnja resolucije, s katero so opisane. Ta hibridni model tekočine ima iste statistične lastnosti kot ustrezen referenčni atomski sistem, v katerem so vse molekule opisane na atomskem nivoju.

V času od 15. do 17. februarja 2006 smo organizirali tridnevni seminar z naslovom: Writing Scientific Papers, ki ga je vodil dr. George W. A. Milne iz National Institutes of Health, Bethesda, Maryland (ZDA), ki je od januarja do septembra 2006 deloval v okviru naše programske in projektne skupine kot uveljavljeni raziskovalec. Seminarja se je vsak dan udeležilo več kot 80 slušateljev. Dr. George W. A. Milne je imel tudi seminarje in predavanja na Inštitutu Rudjer Boškovič v Zagrebu in dvodnevni seminar na Fakulteti za kemijo in kemijsko tehnologijo, Univerza v Ljubljani.

Dr. Dušanka Janežič je urednica (Associate Editor) revije Journal of Chemical Information and Modeling, An American Chemical Society Publications.

Dr. Milan Hodošček je soavtor in razvijalec najbolj uporabljanega računalniškega programa za molekularno modeliranje – CHARMM (Chemistry at HARvard Molecular Mechanics).

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V sodelovanju s firmo Lek d.d., Ljubljana, delamo na projektih raziskav novih učinkovin in na projektih raziskav za obdelavo NMR (jedrska magnetna resonanca) spektrov in molekularnega modeliranja kot pomoč pri interpretaciji NMR spektrov.

Sodelujemo z Inštitutom Jožef Stefan, Medicinsko fakulteto Univerze v Ljubljani, Fakulteto za

tail is sufficient for the rest of the system. The key feature of the new approach is that it allows for a dynamic change in the number of molecular degrees of freedom during the course of an MD simulation by on-the-fly switching between the atomistic and mesoscopic levels of detail. This enables us to reach large length and time scales while spatially retaining atomistic details of the system. The efficiency of the new approach is demonstrated on a model system composed of a liquid of tetrahedral molecules that represents a typical soft matter system, e.g. colloidal system, methane, etc. The simulation box is divided into two regions: one containing only atomistically resolved tetrahedral molecules, the other containing only one particle of coarse-grained spherical molecules. The molecules can freely move between the two regions while changing their level of resolution accordingly. The coarse-grained and the atomistically resolved systems have the same statistical properties.

In the period from 15 to 17 February 2006, we have organized a three day seminar entitled: Writing Scientific Papers, held by Dr. George W.A. Milne of National Institutes of Health, Bethesda, Maryland (USA). The seminar was attended by 80 participants daily. Dr. Milne also held these seminars at the Rudjer Bošković Institute in Zagreb and at the Faculty for Chemistry, University of Ljubljana.

Dr. Dušanka Janežič is an Associate Editor of the Journal of Chemical Information Modeling, An American Chemical Society Publications journal.

Dr. Milan Hodošček is a coauthor and developer of the widely used computer program for molecular modeling – CHARMM (Chemistry at HARvard Molecular Mechanics).

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

In collaboration with Lek d.d., Ljubljana, Slovenia - a recent acquisition of Sandoz, we develop novel chemical entities (NCE's) and we also collaborate on research projects for processing

matematiko in fiziko Univerze v Ljubljani, Biotehniško fakulteto Univerze v Ljubljani, Filozofsko fakulteto Univerze v Ljubljani, Fakulteto za računalništvo in informatiko Univerze v Ljubljani, Univerzo na Primorskem, Koper.

MEDNARODNO SODELOVANJE

Sodelujemo v mednarodni delovni skupini Microsatellite Consortium, ki ga financira Evropska komisija, vodi pa jo prof. David Collier s King's Collegea v Londonu, Velika Britanija.

Kemijski inštitut, Center za molekularno modeliranje in RIKEN Yokohama Institute, High Performance Molecular Simulation Team, Japonska sta podpisala tri letni sporazum o znanstveno raziskovalnem sodelovanju (Collaborative Research Agreement) na področju razvoja namenske strojne in programske opreme za izvajanje simulacij molekulske dinamike bioloških makromolekul. Na slovenski strani je odgovorna nosilka projekta dr. Dušanka Janežič, glavni izvajalec pa dr. Milan Hodošček. Tovrstno sodelovanje potrjuje, da smo med vodilnimi svetovnimi razvijalci vzporednih računalniških gruč za izvajanje vzporednih simulacij molekulske dinamike velikih sistemov, ki jih uspešno uvajamo v Sloveniji in s širokim mednarodnim sodelovanjem tudi slovenskim raziskovalcem omogočamo dostopnost do vrhunske strojne in programske opreme.

Sodelujemo na financiranih bilateralnih projektih, katerih odgovorna nosilka je dr. Dušanka Janežič, z raziskovalci iz naslednjih držav:

- z ZDA, dr. Bernard R. Brooks, National Institutes of Health, Bethesda, MD
- s Hrvaško, dr. Sonja Nikolić, Institut Rudjer Bošković, Zagreb
- s Hrvaško, dr. Sanja Tomić, Institut Rudjer Bošković, Zagreb
- s Turčijo, dr. Gamze Tanoglu, Izmit Institute of Technology, Izmir
- z Romunijo, dr. Mircea Diudea, University of Cluj, Cluj
- z Madžarsko, dr. Istvan Lukovits, Chemical Research Center, Hungarian Academy of Sciences,

NMR spectra using molecular modelling approaches.

We collaborate with Institute Jožef Stefan, Slovenia, Faculty of Medicine, The Faculty of Mathematics and Physics, The Biotechnical faculty, The Faculty of Arts, The Faculty of Computer and Information Science (all members of University of Ljubljana, Slovenia) and University of Primorska, Koper, Slovenia.

INTERNATIONAL COLLABORATION

We collaborate with the international working group, Microsatellite Consortium, which is financed by the European Commission, in the framework of a specific support action coordinated by Prof. David Collier at King's College London, United Kingdom.

National Institute of Chemistry, Center for Molecular Modeling and RIKEN Yokohama Institute, High Performance Molecular Simulation Team, Japan have signed a three year collaborative research agreement on computer hardware and molecular dynamics simulation methods development. The principal investigator in Slovenia is Dr. Dušanka Janežič, and the chief personnel is Dr. Milan Hodošček. Such collaboration proves that we are among the leading developers of parallel computer clusters to be used for molecular dynamics simulations of large systems that we successfully introduced to Slovenia.

We collaborate on financed bilateral projects (Dr. Dušanka Janežič) with researchers from the following countries:

- USA, Dr. Bernard R. Brooks, National Institutes of Health, Bethesda, MD
- Croatia, Dr. Sonja Nikolić, Institut Rudjer Bošković, Zagreb
- Croatia, Dr. Sanja Tomić, Institut Rudjer Bošković, Zagreb
- Turkey, Dr. Gamze Tanoglu, Izmit Institute of Technology, Izmir
- Romania, Dr. Mircea Diudea, University of Cluj, Cluj
- Hungary, Dr. Istvan Lukovits, Chemical Research Center, Hungarian Academy of Sciences, Budapest

es, Budimpešta

POMEMBNI INŠTRUMENTI IN OPREMA

- NMR spektrometri v okviru Slovenskega NMR centra
- FTIR spektrometer Bruker IFS 66S
- PE 2000 NIR Ramanski spektrometer
- izgradili smo vzporedno računalniško gručo VRANA 10, ki jo sestavlja 32x2 AMD Dual-core Opteron 265 procesorjev povezanih z Gigabitnimi stikali.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Dr. George W. A. Milne iz National Institutes of Health, Bethesda, Maryland (ZDA) je bil od januarja do septembra 2006 gostujoči raziskovalec v okviru programske skupine P1-0002.
- Dr. Franci Merzel je bil izvoljen v naziv docenta na Fakulteti za matematiko in fiziko, Univerza v Ljubljani.
- Dr. Matej Praprotnik je na podoktorskem izpopolnjevanju na Max-Planck Institute for Polymer Research v Mainzu, Nemčija.

Mladi raziskovalci (mentorica dr. Dušanka Janežič):

- Urbanu Borštniku je bila odobrena doktorska tema na Fakulteti za računalništvo in informatiko, Univerza v Ljubljani;
- Janezu Koncu je bil odobren direktni prehod na doktorski študij na Fakulteti za farmacijo, Univerza v Ljubljani;
- Nejc Carl je prejel študentsko Prešernovo nagrado na Fakulteti za kemijo in kemijsko tehnologijo, Univerza v Ljubljani.

MAJOR EQUIPMENT

- NMR spectrometers at Slovenian NMR Center
- FTIR spectrometer Bruker IFS 66S
- PE 2000 NIR Raman spectrometer
- We have built the parallel computer cluster, CROW 10 that is composed of 32x2 AMD Dual-core Opteron 265 processors connected with Gigabit Switches.

EDUCATION AND IMPORTANT VISITS

- Dr. George W. A. Milne of National Institutes of Health, Bethesda, Maryland (USA) was a guest researcher from January to September on our program team.
- Dr. Franci Merzel obtained the title "docent" at The Faculty of Mathematics and Physics, University of Ljubljana.
- Dr. Matej Praprotnik is on leave at the Max-Planck Institute for Polymer Research, Mainz, Germany.

Young researchers (mentor Dr. Dušanka Janežič):

- Urban Borštnik's Ph.D. thesis defense was approved at The Faculty of Computer and Information Science, University of Ljubljana,
- Janez Konc's Ph.D. thesis subject was approved at The Faculty of Pharmacy, University of Ljubljana,
- Nejc Carl was awarded the Prešeren students award at the Faculty of Chemistry and Chemical Technology, University of Ljubljana.

L02

Laboratorij za spektroskopijo materialov

Laboratory for Spectroscopy of Materials



VODJA / HEAD
Prof. dr. Boris Orel

RAZISKOVALCI / RESEARCHERS

dr. Zorica Crnjak Orel
dr. Marta Klanjšek Gunde
dr. Angela Šurca Vuk
dr. Lidija Slemenik Perše
dr. Robi Ješe

**MLADI RAZISKOVALCI/
YOUNG RESEARCHERS**

Jelica Vince
Vasko Jovanovski
Mojca Fir
Marko Bitenc
Nina Hauptman
Matjaž Koželj
Ivan Jerman

TEHNIČNO OSEBJE / TECHNICAL STAFF

Helena Spreizer
Petra Jamnik (študentsko delo / student work)



PODROČJA DEJAVNOSTI

Glavni poudarek je bil na razvoju komponent za energetske sisteme, ki izkoriščajo sončno sevanje, in nanokompozitnih materialov za druge aplikacije:

- trdni elektroliti na osnovi kondenziranih ionskih tekočin za Grätzlove fotoelektrokemijske celice in za elektrokromna (pametna) optično preklonna okna;
- večfunkcionalne nanokompozitne prevleke za tekstil, beton in kovine;
- spektralno selektivne barvne prevleke za kolektorske sisteme in fasade;
- nanostrukturne plasti;
- razvoj analzičnih in eksperimentalnih pristopov za raziskave strukture materialov, optičnih lastnosti (barva, termična emisivnost) in površinskih lastnosti (plazemske tehnologije).

BIBLIOGRAFIJA

- 10 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 2 strokovna članka
- 1 poljudni članek

RESEARCH ACTIVITIES

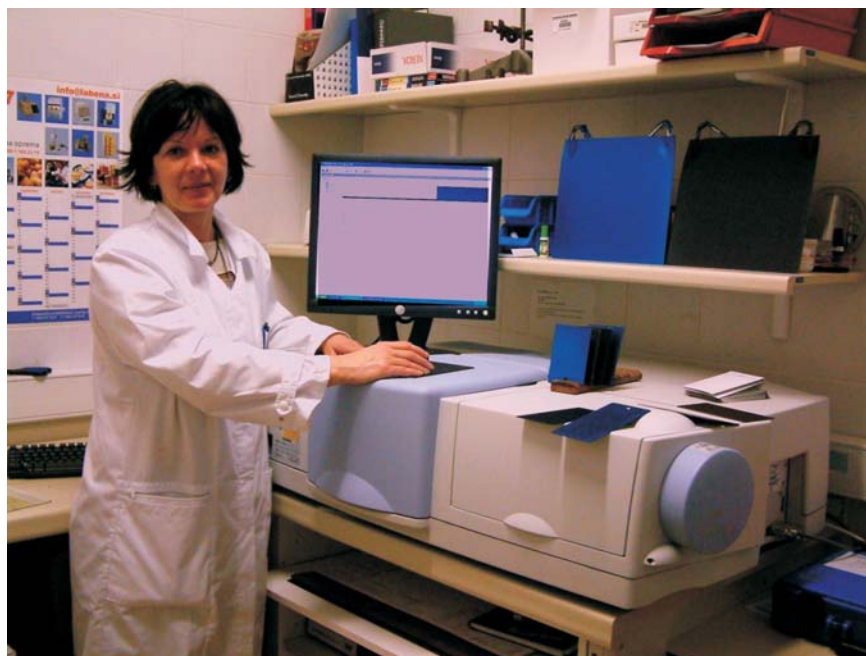
In 2006, we continued with the development of materials for energy systems exploiting solar radiation and nanocomposite materials for other applications:

- solid electrolytes on the basis of condensed ionic liquids for photoelectrochemical Grätzel cells and electrochromic (smart) switchable windows;
- spectrally selective coloured paint coatings for collector systems and facades;
- multifunctional nanocomposite impregnation for textile, concrete and metal;
- nanostructured layers;
- the development of analytical and experimental approaches for the investigation of structure of various materials, optical properties (colour, thermal emissivity) and surface properties (plasma technology).

BIBLIOGRAPHY

- 10 Original Scientific Articles
- 1 Review Article
- 2 Professional Articles

- | | | | |
|----|--|----|--|
| 4 | srednješolski, osnovnošolski ali drugi učbeniki z recenzijo | 1 | Popular Article |
| 3 | priročniki, slovarji, leksikoni, atlasi, zemljevidi | 4 | Reviewed Secondary and Primary School Textbooks or Other Textbooks |
| 4 | objavljeni znanstveni prispevki na konferencah (vabljeni predavanja) | 3 | Manuals, Dictionaries, Lexicons, Atlas, Maps |
| 7 | objavljenih znanstvenih prispevkov na konferencah | 4 | Published Scientific Conference Contributions (Invited Lecture) |
| 1 | objavljeni strokovni prispevek na konferenci | 7 | Published Scientific Conference Contributions |
| 18 | objavljenih povzetkov znanstvenih prispevkov na konferencah | 1 | Published Professional Conference Contribution |
| 2 | objavljena povzetka strokovnih prispevkov na konferencah | 18 | Published Scientific Conference Contribution Abstracts |
| 1 | patentna prijava | 2 | Published Professional Conference Contribution Abstracts |
| 1 | prispevek na konferenci brez natisa | 1 | Patent Application |
| 2 | končni poročili o rezultatih raziskav | 1 | Unpublished Conference Contribution |
| 1 | elaborat, predštudija, študija | 2 | Final Research Reports |
| 2 | diplomi | 1 | Treatise, Preliminary Study, Study |
| 2 | doktorata | 2 | Undergraduate Theses |
| | | 2 | Doctoral Dissertations |



SLIKA 1:
Spektrometer Perkin-Elmer Lambda 950 UV/VIS/NIR.

FIGURE 1:
Spectrometer Perkin-Elmer Lambda 950 UV/VIS/NIR.

GLAVNI DOSEŽKI V LETU 2006

Z nabavo spektrometra Lambda 950 (Perkin-Elmer) smo uspeli v L02 kvalitetno pokriti spektroskopijo materialov v celotnem optičnem področju elektromagnetnega spektra (175 nm – 3300 nm UV-VIS-NIR in 1 mm – 30 mm NIR-IR-Far IR). Tako lahko opravljamo spektroskopske raziskave, ki vključujejo interakcijo elektromagnetnega valovanja z energijo med 7.1 eV in 0.04 eV. Poleg analize številnih snovnih parametrov smo dobili tudi možnost spektroskopskega merjenja absorpcije sončne svetlobe in barvnometričnih lastnosti vzorcev. Tako so se odprle možnosti novih raziskav, za katere smo bili prej znatno vezani na zunanje ponudnike. Spektroskopska znanja v povezavi s poznavanjem snovnih lastnosti so nepogrešljiva pri raziskavah uporabe plazemskih tehnologij. S temi znanji in z učinkovito uporabo vrstične elektronske mikroskopije smo smiselno nadgradili projekte uporabe plazme za obdelavo sodobnih kompozitov na keramični osnovi in za biokompatibilne materiale.

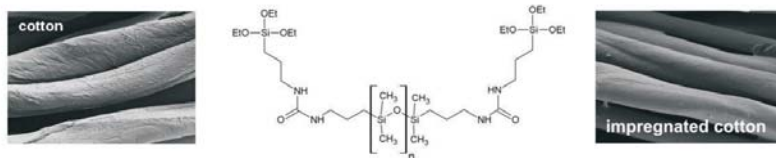
Uporabo metod barvne metrike smo iz premaznih sistemov razširili na barvni videz svetlobe, ki se variabilno spreminja. Tu smo dolgoletno raziskovalno delo laboratorija na področju kromogenih materialov in njihove uporabe za preklopna okna nadgradili z njihovim vplivom na svetlobne razmere v konkretnem ambientu. Problematika odpira opis možnosti variabilne svetlobe za pripravo učinkovitih svetlobnih efektov in za hkratno ustrezno uporabo barv objektov v interieru.

IMPORTANT ACHIEVEMENTS IN 2006

In 2006, we bought a Lambda 950 UV-VIS-NIR spectrophotometer (Perkin-Elmer). This enables us, together with spectrofotometers for the infrared region, to perform advanced spectroscopic studies all over the optical part of the electromagnetic spectrum for wavelengths from 175 nm up to 3300 nm (UV-VIS-NIR) and from 1 mm to 30 mm (NIR-IR-FarIR). The broad spectral region includes interactions of a substance with electromagnetic energy in the region 7.1 – 0.04 eV. It gives us the opportunity to study plenty of different material properties, including solar absorption and colorimetric data evaluation. New research possibilities are therefore opened for the future.

Spectroscopy and broad knowledge of material properties are important in the advanced application of plasma technologies. Together with scanning electron spectroscopy we contribute considerably to the efficient practical use of cold plasma in different types of composites.

The up-to-date methods of colorimetry were successfully applied in a colour rendering study of continuously variable light. Our year-long research of chromogenic materials and its application on switchable windows was expanded to their influence on light properties in the interior of a building with such windows. The currently accomplished research shows possibilities of using variable light for preparing several light-show effects in a simple and energy-



SLIKA 2:

Uporaba hidrofobnih nanokompozitnih materialov za impregnacijo bombažnih tkanin: SEM posnetki neimpregniranih in impregniranih bombažnih vlaken z PDMSU (J. Vince et al., Langmuir, 2006, 22, 6489-6497).

FIGURE 2:

The use of hydrophobic nanocomposite materials for the impregnation of cotton fabrics: SEM micrographs of non-impregnated and impregnated cotton fabrics with PDMSU (J. Vince et al., Langmuir, 2006, 22, 6489-6497).

Poznavanje metod barvne metrike in razmeroma enostavne optike v povezavi z delovanjem očesa je privedlo tudi do razvoja metod za načrtovanje kamuflažnih poslikav na objektih, ki jih želimo zlititi z optičnim vtisom okolice. Te izrazito interdisciplinarne raziskave potekajo v sodelovanju z naravoslovnotehniško fakulteto, Oddelek za tekstilstvo.

Osnova za raziskave nanokompozitov so postopki sol-gel kemije, ki smo jih v letu 2006 razširili na pripravo funkcionaliziranih poliedričnih silseskvioksanov (POSS). Dodatek le-teh v različne polimerne sisteme (selektivne barve, ionske prevodnike ...) izboljšuje njihovo termično stabilnost, trdoto (easy-to-clean prevleke), hidrofobnost in oleofobnost. Z njimi smo uspeli hidrofobizirati tekstil, beton in zaščitili Al-Cu zlitino proti koroziji.

Nadaljevali smo s pripravo nanomaterialov s posebnim poudarkom na doseganju specifičnih morfoloških lastnosti, kot so na primer nanodelci in nanožice, še posebno v povezavi z bakrovimi oksidi.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Color d.d., Medvode; razvoj premazov za sončne zbiralnike in fasade (sodelovanje v okviru Solabs projekta Evropske unije in samostojnega projekta Ministrstva za obrambo Republike Slovenije).
- Fotona d.d., Ljubljana; razvoj nizkoemisivnih kamuflažnih premazov za tanke (sodelovanje v okviru samostojnega projekta Ministrstva za obrambo Republike Slovenije).
- Trimo d.d., Trebnje; Barvni selektivni – energetska učinkoviti premazi za »Solarni panel Trimoterm« (sodelovanje v okviru projekta SEONES – Razvoj sistemov za nizkoenergijske stavbe, 2006–2007).
- Univerza v Ljubljani, Naravoslovnotehniška fakulteta in Tekstina, tekstilna industrija Ajdovščina, d.d.; razvoj večfunkcionalne zaščitne tekstilije za vojaške uniforme (sodelovanje v okviru samostojnega projekta

efficient way. The methods were also proposed to choose suitable colours for objects in the interior.

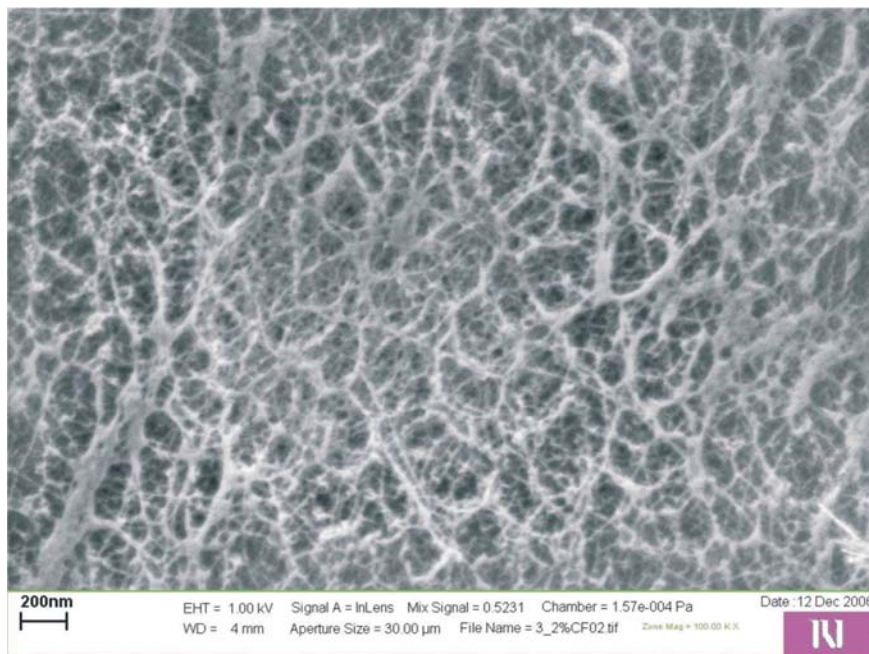
The colorimetric methods, when combined with relatively simplified optical properties of the human eye (to get the optical performance of an average observer) give us some new ideas for developing camouflage patterns. The development of camouflage patterns for a typical urban area is being performed in cooperation with University of Ljubljana, Faculty of Natural Sciences and Technology, Department of Textiles.

The basis for the development of nanocomposite materials are the sol-gel synthesis routes, which in 2006 were expanded on the preparation of functionalised polyedric silsesquioxanes (POSS). Their addition into various polymeric systems (selective paints, ionic conductors...) improved their thermic stability, hardness (easy-to-clean coatings), hydrophobicity and oleophobicity. We succeeded to hydrophobise textile, concrete and Al-Cu alloy with the use of POSS.

We continued with the preparation of nanomaterials with the special stress on the achievement of specific morphological properties as for example, nanoparticles and nanowires, mostly with copper oxides.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Color d.d., Medvode, Slovenia; development of paint coatings for solar collectors and facades (cooperation in the frame of Solabs project of European union and project of the Ministry of Defence in Republic of Slovenia)
- Fotona d.d., Ljubljana, Slovenia; development of low-emitting camouflage paints for tanks (cooperation in the frame of project of the Ministry of Defence in Republic of Slovenia)
- Trimo d.d., Trebnje, Slovenia; Colour selective – energy efficient paints for "Solar panel Trimoterm" (cooperation in the frame of projecta SEONES – Development of Systems for Low-energy Buildings, 2006-2007)



SLIKA 3:

Priprava hidrofobnega premaza za barvne solarne kolektorje z dodatkom nanokompozitov (POSS).

Ministrstva za obrambo Republike Slovenije).

- Center odličnosti »Nanoznanosti in nanotehnologije« (CO NIN – RPR), Nanomateriali v elektrokemijskih sistemih.

MEDNARODNO SODELOVANJE

- Development of unglazed solar absorbers (resorting to coloured selective coatings on steel material) for building facades and integration into heating systems (SOLABS), Št. pogodbe N° ENK6-CT-2002-00679, RTD projekt, 1. 1. 2003 – 30. 6. 2006 (dr. B. Orel).
- Polymer Electrolytes and Non Noble Metal Electrocatalysts for High Temperature Fuel Cells (APOLLON-B), STREP EU projekt, 1. 10. 2006 – 30. 9. 2009 (dr. S. Hočevnar).
- Polymeric Materials for Solar Thermal Applications, International Energy Agency (IAE), sprejet projekt (december 2005), prošnja za pridruženo sodelovanje.

FIGURE 3:

Preparation of hydrophobic polymer resin for solar absorber paint coatings by the addition of nanocomposites (POSS).

- University of Ljubljana, Slovenia, Faculty of Natural Sciences and Engineering and Tekstina, textile industry d.d., Ajdovščina, Slovenia; Development of multifunctional protection for textiles for military uniforms (cooperation in the frame of project of the Ministry of Defence in Republic of Slovenia)
- Centre of excellence "Nanoscience and nanotechnologies" (CO NIN – RPR), Nanomaterials in electrochemical systems

INTERNATIONAL COLLABORATION

- Development of unglazed solar absorbers (resorting to coloured selective coatings on steel material) for building facades and integration into heating systems (SOLABS), Contract N° ENK6-CT-2002-00679, RTD project, 1.1.2003-30.6.2006 (Dr. B. Orel).
- Polymer Electrolytes and Non Noble Metal Electrocatalysts for High Temperature Fuel Cells (APOLLON-B), STREP EU projekt, 1. 10.

- Mreža odličnosti: Nanostructured and Functional Polymer-based materials and Nanocomposites, Proposal No. NOE 500361-2 (dr. Z. Crnjak Orel).
- Raziskave neurejenih materialov: nano optični nanosi, Bilateralno sodelovanje Slovenija–Hrvaška, 2004–2006, Rudjer Bosković (dr. Z. Crnjak-Orel).
- Priprava in karakterizacija uniformnih delcev, Bilateralno sodelovanje Slovenija–ZDA, Clarkson University (dr. Z. Crnjak-Orel).
- Študij strukturnih lastnosti sol-gel materialov z nizko emitivnostjo z IR spektroskopijo, Bilateralno sodelovanje Slovenija–Indija, 10. 10. 2006 – 31. 12. 2007, Central Glass & Ceramic Research Institute, Sol-Gel Division, Kalkuta (dr. Angela Šurca Vuk).
- Sinteze mešanih sistemov na osnovi titanovega oksida: strukturne, elektrokemijske in površinske lastnosti, Bilateralno sodelovanje Slovenija–Italija, 1. 3. 2006 – 31. 2. 2009, University of Trento, Trento (dr. Angela Šurca Vuk).
- CIE, Division 1 (dr. M. Klanjšek Gunde, uradna članica).
- CIE, Division 2, TC2-53 Multi-geometry color measurements of effect materials (dr. M. Klanjšek Gunde, članica).
- CIE, Division 1, TC1-66 Indoor daylight illuminant (dr. M. Klanjšek-Gunde, članica).
- 2006 – 30. 9. 2009 (Dr. S. Hočevar).
- Polymeric Materials for Solar Thermal Applications, International Energy Agency (IAE), accepted project (December 2005), application for associated cooperation.
- Network of excellence: Nanostructured and Functional Polymer-based materials and Nanocomposites, Proposal No. NOE 500361-2 (Dr. Z. Crnjak Orel).
- Development of disordered materials: nano optical coatings, Bilateral cooperation Slovenia-Croatia, 2004-2006, Insitute Rudjer Bošković (Dr. Z. Crnjak-Orel).
- Preparation and characterisation of uniform particles, Bilateral cooperation Slovenia-USA, Clarkson University (Dr. Z. Crnjak-Orel).
- Investigation of structural properties of sol-gel materials with low emissivity with IR spectroscopy, Bilateral cooperation Slovenia-India, 10. 10. 2006 – 31. 12. 2007, Central Glass & Ceramic Research Institute, Sol-Gel Division, Kolkota (Dr. Angela Šurca Vuk).
- Synthesis of mixed systems on the basis of titan oxide: structural, electrochemical and surface properties, Bilateral cooperation Slovenia-Italy, 1. 3. 2006 – 31. 2. 2009, University of Trento, Trento (Dr. Angela Šurca Vuk).
- CIE, Division 1 (Dr. M. Klanjšek Gunde, official member)
- CIE, Division 2, TC2-53 Multi-geometry colour measurements of effect materials (dr. M. Klanjšek Gunde, member)
- CIE, Division 1, TC1-66 Indoor daylight illuminant (Dr. M. Klanjšek-Gunde, member).

POMEMBNI INŠTRUMENTI IN OPREMA

- FT-IR spektrometer Bruker IFS 66/S
- FT-IR in FT-Raman spektrometer Perkin Elmer 2000
- Hewlett-Packard 8453 UV-VIS spektrofotometer z diodnim nizom
- AUTOLAB PGSTAT30 in EG&G PAR 273 potencioestat/galvanostat
- Spektrometer Lambda 950 UV/VIS/NIR

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Robi Ješe: *Strukturne in spektroskopske*

MAJOR EQUIPMENT

- FT-IR spectrometer Bruker IFS 66/S
- FT-IR and FT-Raman spectrometer Perkin Elmer 2000
- Hewlett-Packard 8453 UV-VIS diode-array spectrophotometer

- lastnosti materialov v iono-optičnih sistemih, doktorska disertacija;*
- Mojca Fir: *Sol-gel zaščitne nanokompozitne prevleke za Al-Cu zlitino in sončne absorberje, doktorska disertacija;*
- Daša Šivec: *Vpliv cerija na elektrokromne lastnosti nanokristaliničnih tankih plasti titanovega (IV) oksida, diplomsko delo;*
- Darko Divjak: *Nizkotemperaturna sinteza cinkovih spojin (cinkovega-hidroksid karbonata in cinkovega oksida), diplomsko delo.*

- AUTOLAB PGSTAT30 and EG&G PAR 273 potentiostat/galvanostat
- Spectrometer Lambda 950 UV/VIS/NIR

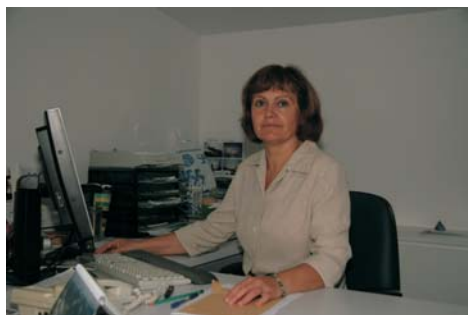
EDUCATION AND IMPORTANT VISITS

- Robi Ješe: Structural and spectroscopic properties of materials in iono-optic systems: Ph.D. dissertation;
- Mojca Fir: Sol-gel protection nanocomposite coatings for Al-Cu alloy and solar absorbers, Ph.D. dissertation;
- Daša Šivec: Influence of cerium on the electrochromic properties of nanocrystalline thin films of titanium (IV) oxide, B.S. thesis;
- Darko Divjak: Low-temperature synthesis of zinc compounds (zinc-hydroxide carbonate and zinc oxide), B.S. thesis.

L03

Laboratorij za kemometrijo

Laboratory of Chemometrics



VODJA / HEAD
Dr. Marjana Novič

RAZISKOVALCI / RESEARCHERS

dr. Marjan Vračko
dr. Neva Grošelj
dr. Marjan Tušar
dr. Natalja Fjodorova (od maja / since may 2006)
dr. Milan Randić (4 mesece / months)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Špela Župerl
Viktor Drgan

RAZISKOVALCI NA DO-DOKTORSKEM DELU IZ TUJINE / YOUNG PRE-DOC SCIENTISTS FROM ABROAD

Andrea Mauri (2 meseca / months)

RAZISKOVALCI NA PO-DOKTORSKEM DELU IZ TUJINE / YOUNG POST-DOC SCIENTISTS FROM ABROAD

dr. Sylwester Mazurek (12 mesecev / months)
dr. Jaroslaw Panek (11 mesecev / months)
dr. Igor Kuzmanovski (5 mesecev / months)



PODROČJA DEJAVNOSTI

Uvajanje kemometrije, to je uporabe široke palete matematičnih, statističnih in računalniških metod za reševanje kemijskih problemov, v raziskovalno in razvojno prakso. Modeliranje kemijskih lastnosti in procesov na področju QSAR študij in iz podatkov, ki jih dobimo s sklopljenimi analiznimi tehnikami.

Uveljavljanje metod umetnih nevronske mreže v kemiji; študij strategij učenja nevronske mreže in razvijanje ustreznih računalniških programov. Raziskave na področju matematične kemije: uporaba diskretne matematike v strukturni kemiji, v QSAR študijah, v proteomiki in genomiki.

Študij algoritmov in razvoj programskih paketov. Uporaba kemometričnih metod v analizni kemiji: zagotavljanje in kontrola kakovosti (QA/QC).

Raziskave 3D reprezentacij kemijske strukture za uporabo v QSAR.

Izobraževanje na področju kemometrije: v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani na diplomskem in podiplomskem nivoju.

RESEARCH ACTIVITIES

- Introduction of chemometrics, i.e. mathematical, statistical and computational methods for solving chemical problems in the applicative, research, and control laboratories
- Modelling of chemical properties and processes in the field of QSAR (Quantitative Structure Activity Relationship) and of data acquired from the hyphenated analytical techniques
- Application of artificial neural network methods in chemistry, study of various ANN learning techniques and development of the corresponding computer software
- Research in the field of mathematical chemistry: the application of discrete mathematics in structural chemistry, in QSAR studies, in proteomics and genomics
- Study of various algorithms and development of computer software
- Application of chemometric methods in analytical chemistry for quality control and quality assurance (QA/QC)

Izobraževanje v okviru posebnih tečajev in šol v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Mariboru.

Izobraževanje in prenos znanja med raziskovalnimi skupinami v raznih državah preko evropskih projektov v Marie Curie izobraževalnih mrežah.

BIBLIOGRAFIJA

- 18 izvirnih znanstvenih člankov
- 3 strokovni članki
- 1 samostojni znanstveni sestavek v monografiji
- 1 samostojni strokovni sestavek v monografiji
- 2 intervjuja
- 6 objavljenih znanstvenih prispevkov na konferencah
- 15 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 prispevek na konferenci brez natisa
- 3 vabljeni predavanja na konferencah brez natisa
- 4 uredništva revij

DOSEŽKI V LETU 2006

- Raziskave, ki smo jih v letu 2006 izvajali sodelavci Laboratorija za kemometrijo, smo predstavili v 16 znanstvenih člankih in dveh poglavjih v monografijah, o rezultatih smo poročali v 12 prispevkih na mednarodnih in 6 prispevkih na domačih znanstvenih konferencah. Objavljena dela kažejo nadaljevanje dela na raziskovalnem programu *Modeliranje relacij med kemijsko strukturo in lastnostjo snovi – QSAR – QSPR* po zastavljenem načrtu.
- Evropski project IBAAC (An Integrated Biomimetic Approach to Asymmetric Catalysis), v katerega smo integrirani kot kemoinformatiki, smo v letu 2006 nadaljevali z enim podoktorskim raziskovalcem, ki je nadaljeval raziskave, začete v prejšnjem letu ter z dvema novima tujima podoktorskima raziskovalcema ter enim doktorantom. Naš cilj je optimizacija katalizatorjev za asimetrično kemijsko sintezo v okolju, ki simulira

- Research of 3D structural structure representations for QSAR
- Education in chemometrics in collaboration with the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia on the pre- and postgraduate levels
- Education in the form of special courses in the collaboration with the Faculty of Chemistry and Chemical Technology, University of Maribor, Slovenia
- Education and knowledge transfer between research groups in several countries on the basis of European Union projects within Marie Curie training networks

BIBLIOGRAPHY

- 18 Original Scientific Articles
- 3 Professional Articles
- 1 Independent Scientific Component Part in Monograph
- 1 Independent Professional Component Part in a Monograph
- 2 Interviews
- 6 Published Scientific Conference Contributions
- 15 Published Scientific Conference Contribution Abstracts
- 1 Unpublished Conference Contribution
- 3 Unpublished Invited Conference Lectures
- 4 Journal Editorships

ACHIEVEMENTS IN 2006

- The research work of the Laboratory of Chemometrics in 2006 is demonstrated in 16 scientific papers and two chapters in the monograph, the results were reported in 12 contributions internationally and 6 at national scientific conferences. The presented work shows the continuation of the progress in the scope of the research program *“Modelling of Structure–property Relationships – QSAR–QSPR”* according to the presumed research plan.
- The European project IBAAC (An Integrated Biomimetic Approach to Asymmetric Cataly-

biološkega (npr. proteini ali dendrimeri, katerih osnovne enote so aminokisljine). O rezultatih smo poročali na sestankih IBAAC projekta v Ljubljani in v Bologni ter na konferencah v Mariboru (Slovenski kemijski dnevi) in v Berlinu (Quantum chemistry – methods and applications). Pomemben sestanek na polovici izvajanja projekta smo organizirali sodelavci Laboratorija za kemometrijo 1. in 2. junija v Ljubljani. Prisoten je bil tudi dr. Sergio di Virgilio iz Evropske unije, ki je zadolžen za spremljanje dela na projektu. Dobili smo pozitivno oceno, kar je bil pogoj za nadaljnje financiranje.

- V evropskem projektu TRACE smo nadaljevali s statistično obravnavo analiznih rezultatov zemlje, vode, oljčnega in lešnikovega olja s pomočjo nevronske mreže. Začetno nalogo, razvoj orodja na osnovi umetne nevronske mreže v MATLAB okolju, smo v prvi različici izvedli ter programe testirali s podatki, ki so na voljo v TRACE-u. Orodje smo razvili do takšne faze, da je primerno za testiranje s katerim koli podatkovnim nizom, urejenim glede na zahteve stare programske opreme, razvite za WINDOWS okolje. O rezultatih smo poročali na sestankih TRACE projekta v Tarragoni, Genovi in v Pragi ter na konferenci v Mariboru (Slovenski kemijski dnevi).
- Aprila 2006 smo začeli z novim evropskim projektom CAESAR (Computer-Assisted Evaluation of industrial chemical Substances According to Regulations). Na prvem sestanku 18. in 19. maja 2006 v Milanu, Italija, smo natančno določili naloge posameznih partnerjev, tako da smo na naslednjem sestanku decembra že lahko poročali o delnih rezultatih. Naša skupina je pripravila podatkovno bazo karcinogenih spojin, izbranih iz raznih javno dostopnih virov, ter po večstopenjskem filtriranju izločila okoli 250 spojin s poznanimi kemijskimi strukturami in določeno stopnjo karcinogenosti. To je osnova za nadaljnje iskanje korelacij med strukturo (popisano s strukturnimi des-

sis), in which we are involved as specialists of chemo-informatics, developed by the integration of two new foreign post-docs and one pre-doc, while one post-doc continued the research he started in the previous year. Our goal is the optimisation of catalysts of asymmetric synthesis in a bio-simulated environment (proteins of dendrimers of amino-acids). We reported the results at the meetings of IBAAC partners in Ljubljana and Bologna, and at conferences in Maribor (Slovenian Chemistry Days) and in Berlin (Quantum chemistry - methods and applications). We were the organizers of an important mid-term meeting in Ljubljana, 1-2 June 2006. It is worthy to note the presence of the European officer, Dr. Sergio di Virgilio, who is responsible for monitoring the progress of the IBAAC project. He was the assessor at the Ljubljana meeting. Being satisfied with the progress, he delivered a report with a positive opinion to Brussels, which was the requirement for further financing.

- Within the TRACE European Union project we continued with statistical evaluation of chemical analyses of earth, water, olive and hazelnuts oil samples with the use of artificial neural networks. The initial task, developing a tool for artificial neural networks in the MATLAB environment, was accomplished through the testing phase. It can be tested for any data providing the suitable input format prescribed in the old WINDOWS software. We reported the results at the TRACE meetings in Tarragona, Genoa, Prague, and in Maribor at Slovenian Chemistry Days.
- In April 2006 we started with a new European project CAESAR (Computer-Assisted Evaluation of industrial chemical Substances According to Regulations). At the first meeting on 18 and 19 May 2006 in Milano, Italy, we browsed through the tasks and assigned short-term goals for each participant group. At the next meeting we already reported on partial results. Our group was responsible for

kriptorji) in lastnostjo, stopnjo karcinogenosti, kar končno vodi h klasifikacijskemu ali napovednemu modelu.

- V letu 2006 smo izvajali dva industrijska projekta. Prvi je BIO11/2006, v katerem nadaljujemo v prejšnjem letu začeto ovrednotenje podobnosti/identičnosti kemijskih struktur nekaterih učinkovin, ki jih raziskuje farmacevtska družba Lek Pharmaceuticals, d.d., Ljubljana. Drugi je projekt s podjetjem IMS-ADITOIL d.o.o., Trzin, pogodba št. 120/06-L03 o dolgoročnem sodelovanju na področju raziskav in razvoja nizko temperaturnih bitumnov in asfaltnih zmesi. V okviru pogodbe sodelavci Kemijskega inštituta opravljamo temeljne in aplikativne raziskave, razvijamo analitske metode, pripravljamo ekspertna mnenja, skupaj z IMS-ADITOIL d.o.o. pripravljamo projekte in predstavitve za strokovno javnost o nizko temperaturnih bitumnih in asfaltnih zmesih.

- V okviru sodelovanja s Skupnim raziskovalnim centrom (European Chemical Bureau, Institute for Health and Consumer Protection, Joint Research Centre, Ispra, Italija) je sodelavec (dr. Marjan Vračko), ki je marca zaključil enoletno bivanje kot gostujoči znanstvenik (Senior Scientist Visitor), predstavil nevronske mreže kot ustrezno orodje za postavitev QSAR modelov, ki so uporabni za regulacijske namene. V reviji SAR&QSAR Environ. Res. smo skupaj s strokovnjaki iz ECB objavili članek o validaciji protitočnih (counter-propagation) nevronskih mrež v luči OECD principov validacije QSAR modelov, ki se uporabljajo za regulacijske namene. Dokument je dostopen na spletni strani OECD:

<http://www.oecd.org/dataoecd/55/35/38130292.pdf>

Poleg tega smo bili aktivni na področju razvoja kemometrijskih metod in aplikacij in na področju teorije grafov z uporabo v strukturnih reprezentacijah, v proteomiki in genomiki, kot je razvidno iz bibliografije.

a compiling a carcinogenicity data base from open public sources. After several filterings we selected cca. 250 compounds with known chemical structures and ascribed their carcinogenicity. On this basis a further search for the relationship between chemical structure and carcinogenicity will be carried out, with the aim of obtaining the classification and predictive models.

- Two industrial projects were going on in 2006. The first one, BIO11/2006, is a continuation of the project started in the previous year, in which we were evaluating the similarity/identity of molecular structures of drugs investigated by Lek Pharmaceuticals, d.d., Ljubljana, Slovenia. The second project with the company IMS-ADITOIL d.o.o., Trzin, Slovenia; contract no. 120/06-L03, was for long-term collaboration in the field of research and development of low temperature bitumen and asphalt mixes. In the frame of this contract, researchers for the National Institute of Chemistry work on basic and applicative research, develop analytical methods, prepare expert studies; in collaboration with IMS-ADITOIL d.o.o. we apply for projects and prepare presentations about low temperature bitumen and asphalt mixes for the public in the field of road construction.
- In March 2006, one of our co-workers (Dr. Marjan Vračko) finished his appointment as the senior scientist visitor in the European Chemical Bureau, Institute for Health and Consumer Protection, Joint Research Centre (JRC), Ispra, Italy. In our contribution to the work of JRC we presented the counter propagation neural networks as a suitable tool for QSAR modelling. In the journal SAR&QSAR Environ. Res. we published, together with invited experts the article, research on validation of counter propagation neural networks in terms of OECD principles for validation of QSAR models used for regulatory purposes. The document is available on the OECD website:

- V letu 2006 smo podpisali Sporazum o dolgoročnem sodelovanju z Univerzo v Trstu, (Biophysics and Macromolecular Chemistry (BBCM)). Sporazum temelji na skupnih raziskovalnih interesih Oddelka za biokemijo, biofiziko in makromolekularno kemijo Univerze v Trstu (profesorica dr. Sabina Passamonti) in Laboratorija za kemometrijo KI (dr. Marjana Novič). K sporazumu so prispevale skupne raziskave o delovanju proteinskih transporterjev (bilitranslokaze), ki so bile med drugim rezultat trimesečnega bivanja naše mlade raziskovalke v njihovem laboratoriju, kar je omogočilo, da so bili teoretični izračuni nadgrajeni z eksperimentalnimi rezultati.
- Pod mentorstvom naših sodelavcev in v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani sta dva mlada raziskovalca nadaljevala doktorsko izobraževanje. Enemu od njih je bil na osnovi doseženih rezultatov že odobren direkten prehod na doktorat brez magisterija, drugi bo za prehod zaprosil naslednje leto.

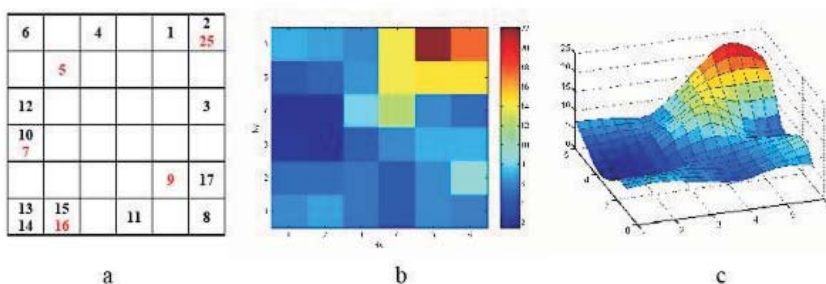
KRATEK OPIS DELA IN REZULTATOV

Glavnino raziskav smo opravili v okviru financiranja raziskovalnega programa P1-017, *Modeliranje relacij med kemijsko strukturo in lastnostjo snovi – QSAR – QSPR*. Raziskovalna

<http://www.oecd.org/dataoecd/55/35/38130292.pdf>

Other activities, mainly in the field of development and application of chemometrics methods and in the field of graph theoretical descriptors for proteomics and genomics, are apparent from the bibliography.

- In 2006, we signed an agreement for long term collaboration with the Biophysics and Macromolecular Chemistry (BBCM) Department of University of Trieste, Italy. The agreement is based on the common research interest of BBCM (Prof. Sabina Passamonti) and our group in the Laboratory for Chemometrics (Dr. Marjana Novič). The basis for the agreement was collaboration on the research of mechanism and structural details of protein transporters (bilitranslocase), which, among other things, resulted in a three month stay of our young researcher in their laboratory. This collaboration linked our theoretical approach with their experimental results.
- Under the mentorship of our co-workers and in collaboration with Faculty of Chemistry and Chemical Technology of the University of Ljubljana, Slovenia, two Ph.D. students are continuing with their education. On the basis of the results one was allowed to work



SLIKA:

Vrhnja mapa 6 x 6 nevronov (a), ravnina odgovorov (b) in 3D pogled na ravnino odgovorov (c) napovednega modela na osnovi protitočne nevronske mreže, trenirane s petnajstimi spojinami iz družine flavonoidov.

FIGURE:

Top-map of 6x6 neurons (a), response surface (b), and 3D view on the response surface (c) of a predictive model based on counter propagation of an artificial neural network trained with fifteen flavonols.

tematika programa nam omogoča vrsto mednarodnih povezav in vključitev v evropske in domače industrijske projekte. Del raziskav, ki jih posvečamo razvoju in uporabi topoloških indeksov ter uporabe teorije grafov, je objavljeno v devetih publikacijah v sodelovanju z mnogimi strokovnjaki teoretsko-matematičnega področja. Nosilni steber tovrstnih raziskav, profesor Milan Randić, se je tudi to leto pridružil naši raziskovalni skupini za daljše časovno obdobje. Skupne raziskave imajo rezultate, kar je razvidno iz objav v publikacijah, v katerih se pokaže tudi praktično uporabna vrednost graf-teoretičnih invariant, predvsem na QSAR področju. Nadaljevali smo z matematičnim pristopom analize podatkov v proteomiki in genomiki. V sodelovanju z Zavodom za zdravstveno varstvo Maribor (ZZVMB) smo zaključili študijo kvalitete voda različnih vodnjakov. Nadaljujemo s spremljanjem prisotnosti pesticidov metolaklor in njegovih razgradnih produktov v površinskih vodah. Metolaklor, selektivni herbicid za zatiranje določenih vrst trave in širokolistnega plevla, se zaradi polarnega značaja izpira s površine in je prisoten v vodnih vzorcih, poleg tega pa tudi metabolira, zato je spremljanje metabolitov še posebej pomembno, če želimo dobiti sliko onesnaženja.

Aktivno smo se vključili v delovanje centra SENARC (Slovenian European Natural Research Centre), in sicer na poletni šoli v Mariboru, 3. – 14. julija 2006, kjer smo se odzvali na vabila in imeli tri predavanja (Uvod v analizo podatkov z več spremenljivkami, Izbrana poglavja iz kemometrije in Vloga QSAR modelov in kemometrijskih metod v evropski zakonodaji). Namen poletne šole je bil zbrati podiplomske študente iz zahodnih balkanskih držav na uvodnem tečaju o problemih, povezanih z meritvami, ter praktičnem usposabljanju v laboratoriju, da bi s tem vzpostavili nadaljnje sodelovanje v raziskavah. Naslednji dogodek, v katerem smo sodelovali, je bil v Lipici 26. – 27. septembra 2006 (12. mednarodni simpozij o separacijskih tehnikah), in sicer smo prispevali

directly towards his Ph.D. without first obtaining a Master degree. The other will apply for passing the next year.

SHORT DESCRIPTION OF RESEARCH AND RESULTS

The majority of the research work was accomplished in the financing frame of the research program P1-017, *Modelling of Structure–property Relationships – QSAR–QSPR*. The subject matter of the research project enables us to maintain many international collaborations and to integrate with several European and domestic industrial projects. The results of the research directed towards graph theory and investigation of topological indices are presented in 9 papers in collaboration with many theoreticians from different parts of the world. The protagonist of this kind of research is professor Milan Randić, who is joining us for a full year. From the attached bibliography one can see that published results of common research work demonstrate the practical application of graph-theoretical invariants, especially in the field of QSAR modelling. We continued with the mathematical approach in analysis of data from proteomics and genomics. In collaboration with the Institute of Public Health Maribor, Slovenia (IPHMB), we completed the study of water quality from different water wells. We continue monitoring metalachlor and degradation products in surface waters. Metolachlor, a selective herbicide used to control specific annual grasses and broadleaf weed and is leachable into the groundwater due to its highly polar characteristics, so it is present in water samples. Additionally, it metabolises, so the monitoring of metabolites is of special importance if we want to obtain the pattern of pollution.

We were actively involved in the endeavours of SENARC, (Slovenian European Natural Research Centre) with three invited lectures at Summer School in Maribor, 3 – 14 July 2006: *Introduction to Multivariate Analysis, Selected Topics from Chemometrics, and The Role of QSAR Models and Chemometrical Methods in Euro-*

k organizaciji in izvedbi delavnice o pripravi vzorcev in validaciji.

Poseben poudarek velja širitvi sodelovanja našega laboratorija z industrijo. Poleg podaljšanja projekta s farmacevtsko družbo Lek Pharmaceuticals, d.d., Ljubljana (BIO11/2006) smo uspeli podpisati novo pogodbo o dolgoročnem sodelovanju s podjetjem IMS-ADITOIL d.o.o., Trzin, (120/06-L03). V prvem primeru gre za nadaljevanje prejšnje leto začelih raziskav v smislu ovrednotenja podobnosti/identičnosti kemijskih struktur nekaterih učinkovin v zdravilih (generikov), ki jih raziskuje farmacevtska družba Lek Pharmaceuticals. V nadaljevanju so v L11 pripravili nove preparate z dodatki, ki bi čim bolj izenačili novi proizvod z originalnim zdravilom. Naša naloga je bila ovrednotiti podobnosti 2D NMR spektrov posameznih izolatov z različnimi dodatki. Rezultati dela so zbrani v članku, ki smo ga poslali v objavo, ter v predstavitev na konferencah. Drugi projekt, Raziskave in razvoj nizko temperaturnih bitumnov in asfaltnih zmesi za IMS-ADITOIL, je namenjen temeljnim in aplikativnim raziskavam, razvijanju analitske metode, pripravljanju ekspertnih mnenj, pripravljanju projektov in predstavitev za strokovno javnost o nizko temperaturnih bitumnih in asfaltnih zmesih. V okviru navedene pogodbe smo na Kemijskem inštitutu v letu 2006 izvedli naslednje dejavnosti:

- (i) za Dneve občinskih cest smo pripravili predstavitev z naslovom *Uporaba nizkotemperaturnih asfaltov na občinskih cestah, parkiriščih, pločnikih in dvoriščih* (5. maja 2006), kjer je bila za ciljno publiko (občinski investitorji in izvajalci) poudarjena raba nizko temperaturnih bitumnov in asfaltnih zmesi na manj obremenjenih površinah. Poudarjeno je bilo, da nizkotemperaturne asfalte zmesi omogočajo daljši čas med proizvodnjo in vgradnjo, kar je pomembno pri oskrbovanju več manjših gadbišč. Prometne površine lahko tudi po vgradnji takšnih asfaltnih zmesi hitreje predamo prometu.
- (ii) Na DARS-ov razpis razvojno raziskovalnih nalog je bila poslana ponudba z naslovom

pean Chemical Legislation. The aim of the Summer School was to bring together post-graduate students from the Western Balkan Countries to initiate further research collaboration by an introductory course on measurements, related issues and hands-on training. The next event in which we participated as experts from SENARC centre was in Lipica: 12th International Symposium on Separation Sciences, 27 - 29 September 2006, in particular focusing on organization and implementation of the workshop on sample preparation and validation methods.

A special emphasis should be given to the extended collaboration of our laboratory with the industry. Apart from the prolongation of the previously started project with Lek Pharmaceuticals, d.d., Ljubljana, Slovenia (BIO11/2006), we succeeded in a new long term collaboration agreement with the company IMS-ADITOIL d.o.o., Trzin, Slovenia (120/06-L03). In the first case we continued with the evaluation of similarity/identity of molecular structures of drugs in biopharmaceuticals being investigated by Lek Pharmaceuticals, d.d. In L11 new isolates with various additives were prepared in order to identify and eliminate the difference between the new isolates and original drug. Our task was to evaluate the similarity of 2D NMR spectra of individual isolates with different additives. The results were reported in a manuscript, sent for publication by the end of the year and demonstrated at international scientific conferences. The second project, research and development of low temperature bitumen and asphalt mixes for IMS-ADITOIL d.o.o., encompasses the basic and applicative research, development of analytical methods, preparation of expert studies, applications for projects, and presentations about low temperature bitumen and asphalt mixes for the public in the field of road construction.

In the framework of this contract the following activities were completed:

- (i) For a meeting called "Dnevi občinskih cest" we prepared a presentation with title: "Use

Nizkotemperaturni asfalti in ohranitev nizkotemperaturnih lastnosti pri reciklaži (14. junija 2006). Pri nalogi smo nameravili razviti analitske metode, ki bi omogočale kvantitativno določevanje nizkotemperaturnega dodatka v recikliranih asfaltnih zmesih. Naloga ni bila sprejeta iz povsem formalnih razlogov.

(iii) Referat z naslovom *Nizko temperaturna bitumenska veziva* je bil predstavljen na 8. kongresu o cestah in prometu v Portorožu (26. oktobra 2006). V zborniku je bil predstavljen tudi prispevek v obliki članka. V referatu so bili zbrani vsi podatki o vgradnji nizko temperaturnih asfaltnih zmesi na testnih poljih v Sloveniji ter tudi predstavljeni podatki o prihranku pri energiji, zmanjšanju emisije toplogrednih plinov pri proizvodnji ter emisije bitumenskih hlapov pri vgradnji.

(iv) Pri vgrajevanju nizkotemperaturnega asfalta v Luki Koper je bil opravljen strokovni ogled, pripravili smo poročilo o ogledu ter podali tudi priporočila izvajalcem (10. novembra 2006). Ob tej priliki so bili odvzeti vzorci bitumna in asfalta. Na teh vzorcih so bile izvedene preiskave na ZAG-u, na Kemijskem inštitutu pa spektroskopska preskušanja še potekajo.

(v) V skladu z dogovorom z gospodom Aljošo Lipovškom, direktorjem podjetja SCT Finalna dela, Ljubljana, je bil napisan predlog projekta z naslovom *Študija vplivov nizkotemperaturnih dodatkov v litem asfaltu na okolje*, ki bo predvidoma poslan na razpis Ministrstva za gospodarstvo. Pri vgradnji litih asfaltov je zahtevana še višja temperatura, kar vodi še do večje emisije bitumenskih hlapov. Ker je vgradnja litega asfalta izvedena ročno, lahko z znižanjem temperature veliko prispevamo k zdravstveni zaščiti vgrajevalcev.

Bilateralni projekt med ZDA in Republiko Slovenijo z naslovom *Avtomatična primerjava in ovrednotenje proteomičnih podatkov* smo realizirali v obliki daljšega obiska ameriškega sodelavca dr. Sola Bobsta v Sloveniji (6 tednov)

of low temperature asphalt mixes on low volume roads, parking places, paved footways and backyards" (5 May 2006). For the target audience (local investors and contractors) main stress was put on use of low temperature asphalt mixes on less trafficked pavements. It was emphasized that with low temperature asphalts a contractor has more time between productions and build in; that is more important when the producer of asphalt has to supply many small construction places. When using low temperature asphalt mixes pavements can be more quickly opened to traffic;

(ii) On a public official invitation for R&D studies from DARS (Highway agency, Ljubljana, Slovenia) we sent an offer for a project entitled: "Low temperature asphalt mixes and preservation of low temperature asphalt properties in the recycling process" (14th June.2006). In this project we intended to develop analytical methods for quantitative determination of low temperature additive in recycled asphalt mixes. Project was not accepted due to formal reasons;

(iii) A lecture with title "Low temperature bitumen binders" was orally presented at the 8th Slovene road congress in Portorož (26 October 2006). In the conference proceedings also an article was published, in which we collected all information about building in low temperature asphalt mixes in Slovenia, i.e. test fields, energy savings, reduction of Greenhouse gas emission at production and emission of bitumen fumes in building in low temperature asphalts;

(iv) For laying low temperature asphalts in the Port of Koper, Slovenia we prepared a report based on an inspection of work. This report also included recommendations for constructors (10 November 2006). During inspection samples of bitumen and asphalt were taken. On these samples some analyses were performed in the National Institute of Building and Civil Engineering and the National Insti-

ter krajšega obiska dveh sodelavcev L03 (dr. Marjana Novič, dr. Marjan Vračko) v ZDA. Dr. Sol Bobst je med šesttedenskim bivanjem v Sloveniji pripravil okolje za pregledovanje in shranjevanje javno dostopnih proteomskih map na osebem računalniku. Naredili smo tudi nekaj testnih študij (rokopis članka je v pripravi), s pomočjo katerih bomo prikazali možnost uporabe proteomskih podatkov v regulatorne namene. Obisk obeh slovenskih raziskovalcev v ZDA (The McKim Conference on the Use of QSARs and Aquatic Toxicology in Risk Assessment, 27. – 29. junij 2006) je bil namenjen ravno proučevanju možnosti uporabe proteomike v ameriški agenciji za zaščito okolja (EPA). V okviru slovensko-indijskega bilateralnega projekta: *QSAR protituberkuloznih učinkovin, primerjava modelov nevronske mreže in linearnih modelov* smo izvedli dva obiska. Aprila je na Kemijskem inštitutu gostoval prof. Manish Bagshi z Indijskega inštituta za kemijsko biologijo (Indian Institute of Chemical Biology), v decembru je dr. Marjan Vračko obiskal omenjeni inštitut v Kalkuti. Študirali smo niz 37 quinoksalskih spojin in njihovo aktivnost proti bakteriji *Mycobacterium tuberculosis*. Primerjali smo linearne in modele nevronske mreže. Modele nevronske mreže smo uporabili tudi za klasifikacijo omenjenih spojin. V pripravi sta dva rokopisa.

Omeniti velja še doprinos naše raziskovalne skupine k IBAAC projektu, ki je v letu 2006 dosegel največjo intenziteto (štirje tuji doktorski in podoktorski sodelavci). Nadaljevali smo s prakso, da gredo raziskovalci, ki se vključijo v IBAAC projekt kot doktoranti ali podoktoranti, najprej za določen čas (1–3 mesece) v laboratorij enega od partnerjev, kjer se seznanijo s problematiko organske biokatalize, ter potem nadaljujejo z raziskavami v našem laboratoriju. Tako je bil letos eden od podoktorantov pri švicarskem partnerju IBAAC projekta, profesorju Thomasu Wardu na Univerzi v Neuchatelu, drugi pa na Univerzi v Bernu pri profesorju Jean-

tute of Chemistry;

- (v) In agreement with Mr. Aljoša Lipovšek (director of SCT Final works, Ljubljana, Slovenia) we prepared a project "Study of low temperature additives in mastic asphalt on the environment". When laying mastic asphalt, even higher temperatures are needed and emissions of bitumen fumes are higher than for ordinary asphalts. Due to the fact that building with mastic asphalt is done manually, the health risk to workers is better prevented when using low temperature additives.

The bilateral project between the USA and R Slovenia entitled *Proteomics Data for Automatic Comparison and Evaluation* was realised in the sense of a longer visit (6 weeks) by the American principal investigator, Dr. Sol Bobst in Slovenia and two shorter visits of Slovenian investigators (Dr. Marjana Novič, Dr. Marjan Vračko) in the USA. During his stay in Slovenia Dr. Sol Bobst prepared the computer environment (PC) for browsing and storing publicly available proteomic maps. We also performed some test studies (the manuscript is in preparation), which would show the suitability of proteomics data for regulatory purposes. The visit of the Slovenian scientists in the USA (The McKim Conference on the Use of QSARs and Aquatic Toxicology in Risk Assessment, June 27–29, 2006) was meant to evaluate how similar activities are adopted by the US Environmental Protection Agency (EPA).

In the framework of the Slovenian-Indian bilateral cooperation project entitled: *QSAR of Antituberculosis Drugs: A Comparison of Statistical and Neural Net Methods*, we completed two visits. In April 2006, Prof. Manish Bagshi from the Indian Institute of Chemical Biology visited KI, and in December 2006, Dr. Marjan Vračko visited the institute in Calcutta. We studied the set of 37 quinoxaline compounds and their activities against *Mycobacterium tuberculosis*. We compared linear models and counter propagation neural network models, which

Louis Reymond. Eden od obeh je šel še na enomesečno specializacijo iz kvanto-mehaničnih računov v Wisconsin, Minnesota, k profesorju Qiang-u Cui-u. Prvi del kemoinformacijske kompleksne raziskave sistema »Avidin/Streptavidin – biotiniran ligand« je zaključen in pripravljen za objavo, medtem ko so preliminarni rezultati v letu 2006 objavljeni v dveh revijah z visokim faktorjem vpliva (JACS in Inorg. Chem.).

Plod sodelovanja z Univerzo v Trstu, Italija, je objava raziskave delovanja bilitranslokaze, proteina, ki je odgovoren za transport bilirubina (in drugih molekul) skozi celično membrano v jetrih. Naš namen je bil osvetliti način interakcije flavonoidov z bilitranslokazo. Ugotovili smo, da vezavna interakcija temelji na sposobnosti tvorbe vodikovih vezi, kar zmanjšuje pomen interakcij nabitih delov molekule. Posebno pozornost smo posvetili izboru molekularnih deskriptorjev, potrebnih za izgradnjo modela. Rezultati te raziskave kažejo, da večina flavonolov, prisotnih v hrani, za razliko od antocianov ne reagira z bilitranslokazo, medtem ko se nekateri aglikoni šibko vežejo. Kvantitativna analiza povezave med molekularno strukturo in sposobnostjo vezave je vodila k identifikaciji tistih delov molekule, ki so potencialno odgovorni za vezavne interakcije z bilitranslokazo, ter nam omogočila postaviti hipotezo o mehanizmu vezave med ligandom in proteinom.

SODELOVANJE Z INDUSTRIJO

- Lek Pharmaceuticals, d.d., Ljubljana; projekt BIO11/2006
- IMS-ADITOIL d.o.o., Trzin; pogodba št. 120/06-L03

POTENCIALNI INDUSTRIJSKI UPORABNIKI

Laboratoriji za kontrolo in zagotavljanje kvalitete v vseh vejah kemijske (in druge) predelovalne industrije, v katerih lahko z metodami načrtovanja eksperimentov in

were additionally used for classification of compounds. Two manuscripts are in preparation.

It is worth mentioning the contribution of our research group to the European Union project IBAAC, which culminated in 2006 with four foreign post-docs and post graduate students. We continued with the practice that fellows spend a shorter period in an experimental laboratory for organic catalysis with one of our project partners to become acquainted with the subject of the project (bio-catalysis). Then they continue with the chemo-informatics part in our group. In 2006, one of the post-docs was in Bern with Professor Thomas Ward at the University of Neuchatel, while the other was at the University of Bernu with Professor Jean-Louis Reymond. One of them made a one-month specialisation on quantum-mechanical calculations at the University of Wisconsin, Minnesota, with Professor Qiang Cui. The first part of a complex chemo-informatics investigation of the system "Avidin/Streptavidin – biotinilated ligands" is completed and ready for publishing, while the preliminary results were published in 2006 in two journals with high impact factors (JACS and Inorg. Chem.).

Our collaboration with the University of Trieste, Italy, resulted in a common publication on the investigation of the transport mechanism of bilitranslocase, the membrane protein responsible for transport of bilirubin from liver cells to the blood. Our purpose was to shed light on the nature of flavonoid interaction with bilitranslocase. It was found that binding relies on the ability to establish hydrogen bonds, ruling out the involvement of charge interactions. Special attention was dedicated to the examination of the kind of molecular descriptors needed to create the model. The results of this work show that, contrary to dietary anthocyanins, most dietary flavonols do not interact with bilitranslocase, whereas, some flavonol aglycones act as poor ligands of that carrier. The quantitative analy-

modeliranjem lastnosti večkomponentnih izdelkov bistveno skrčimo drago in težavno eksperimentalno delo ter tako pocenimo izdelke in izboljšamo njihovo kvaliteto.

MEDNARODNO SODELOVANJE

Mednarodni projekti:

- projekt TRACE (FP6-2003-FOOD-2-A) (*Tracing Food Commodities in Europe*). (Contract No. TRACE-IP-006942);
- projekt IBAAC (*An Integrated Biomimetic Approach to Asymmetric Catalysis*) (Contract No. MCRTN –CT-2003-505020);
- projekt CAESAR (*Computer-Assisted Evaluation of industrial chemical Substances According to Regulations*) (SSPI-022674);
- projekt COST D2 (*New fluororous media and processes for cleaner and safer chemistry;*)
- bilateralni projekt v okviru slovensko-indijskega programa znanstveno tehnološkega sodelovanja 2004–2006 z naslovom: *QSAR protituberkuloznih spojin: primerjave statističnih modelov in nevronskih mrež*. Nosilca: dr. Marjan Vračko in dr. Manish Bagshi;
- bilateralni projekt v okviru znanstveno-tehnološkega sodelovanja med Republiko Slovenijo in Republiko Makedonijo v letih 2004, 2005 in 2006 z naslovom: *Študij relacij med kemijsko strukturo in aktivnostjo molekul, ki inhibirajo HIV-1*. Nosilca: dr. Marjana Novič in dr. Igor Kuzmanovski;
- bilateralni projekt v okviru znanstveno-raziskovalnega sodelovanja med Republiko Slovenijo in Združenimi državami Amerike v letih 2006–2007 z naslovom: *Avtomatična primerjava in ovrednotenje proteomičnih podatkov*. Nosilca: dr. Marjana Novič in dr. Sol Bobst. (BI-US/06-07-013).

POMEMBNEJŠI INŠTRUMENTI IN DRUGA OPREMA

- računalniška učilnica s 30 sedeži in 16 osebnimi računalniki;

sis of the structure–activity relationship led to the identification of parts of ligands potentially involved in the binding to bilitranslocase, along with a reliable hypothesis on the kind(s) of interaction between the ligand and the target.

COLLABORATION WITH THE INDUSTRY

- Lek Pharmaceuticals, d.d., Ljubljana, Slovenia; Project BIO11/2006
- IMS-ADITOIL d.o.o., Trzin, Slovenia; Contract no. 120/06-L03

POTENTIAL INDUSTRY PARTNERS

Quality assurance and quality control laboratories in all branches of chemical, pharmaceutical and other kind of secondary industry, in which the application of experimental design, modelling and optimization techniques one can reduce the expensive and tedious experimental work and thus lower the prize and improve quality of products.

INTERNATIONAL COLLABORATION

Projects:

- Project TRACE (FP6-2003-FOOD-2-A) (*Tracing Food Commodities in Europe*). (Contract No. TRACE-IP-006942)
- Project IBAAC (*An Integrated Biomimetic Approach to Asymmetric Catalysis*) (Contract No. MCRTN –CT-2003-505020)
- Project CAESAR (*Computer-Assisted Evaluation of industrial chemical Substances According to Regulations*) (SSPI-022674)
- Project COST D2 (*New fluororous media and processes for cleaner and safer chemistry*)
- Bilateral projects in the frame of 'Slovenian-Indian intergovernmental science and technology cooperation programme for the period 2004 - 2005' entitled 'QSAR of antituberculosis drugs: A comparison of statistical and neural nets models'. Principal investigators are dr. Marjan Vračko and dr. Manish Bagshi.
- Bilateral projects in the frame of 'Scientific and technological cooperation between R

- DIONEX-DX500 ionski kromatograf z novim avtomatskim vzorčevalnikom

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Kot vsako leto smo tudi letos povabili na trimesečni delovni obisk profesorja Milana Randića, uveljavljenega raziskovalca na področju teorije grafov, ki je že več let zunanji sodelavec naše programske skupine. V letu 2006 smo tudi uspešno konkurirali na javnem razpisu za (so)financiranje uveljavljenih raziskovalcev iz tujine, tako da smo za obisk profesorja Randića dobili dodatna sredstva in na tej osnovi je začetni obisk (maj – september 2006) dopolnil s krajšim obiskom v decembru, kar nam je omogočilo končati delo (rokopis), začeto med prvim obiskom.

Mlada raziskovalka Špela Župerl je bila tri mesece na dodatnem doktorskem izpopolnjevanju v Italiji pri dr. Sabini Passamonti (na Univerzi v Trstu, Italija, na Oddelku za biokemijo, biofiziko in kemijo makromolekul). Namen usposabljanja je bilo spoznavanje mehanizmov prenosa učinkovin v celice. Te raziskave so vključene tudi v predlogu teme doktorske disertacije.

Slovenia and R Macedonia for the period 2004 - 2006' entitled 'Quantitative Structure-Activity Relationship Studies of HIV-1 Inhibitor Molecules' Principal investigators are dr. Marjana Novič and dr. Igor Kuzmanovski.

- Bilateral project in the framework of scientific between Republic of Slovenia and United States of America in the years 2006 – 2007', entitled "*Proteomics data for automatic comparison and evaluation*". Principal investigators are Dr. Marjana Novič and Dr. Sol Bobst. (BI-US/06-07-013).

IMPORTANT INSTRUMENTS

- Computer supported class-room with 30 seats and 16 PCs;
- DIONEX-DX500 ion chromatograph with new auto sampler.

EDUCATION AND IMPORTANT VISITS

Professor Milana Randić, recognized researcher in the field of graph theory, was invited for a 4-months research visit to our group. He is an external collaborator of our research program P1-017 for a longer period. In 2006 we successfully applied for funding of his visit, call of ARRS for (co)financing visits of eminent foreign researchers. On this basis with additional funding professor Randić completed his stay with a second visit in December, which enabled us to finish the paper work of the research activities started during the first visit.

Young researcher Špela Župerl was on a three-month doctoral specialization with professor Sabina Passamonti, in the Biophysics and Macromolecular Chemistry (BBCM) Department of University of Trieste, Italy. The purpose of her specialization was to get insight into the experimental part of investigation of mechanisms of transport through the cell membrane. This subject is included in the proposal of her doctoral thesis.

L04

Laboratorij za analizno kemijo

Analytical Chemistry Laboratory



VODJA / HEAD

Dr. Božidar Ogorevc

RAZISKOVALCI / RESEARCHERS

dr. Bojan Budič
dr. Johannes T. van Elteren
dr. Irena Grgič
dr. Samo Hočevar
dr. Miroslav Kovačevič (do / until 14. 5.)
doc. dr. Milko Novič
dr. Janja Turšič (dopolnilno delovno razmerje /
part time)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Marija Slavec
Lea Mauko
Mersida Janeva (od novembra / from november)
Darja Kotnik (od novembra / from november)
Petra Apat (od oktobra / from october)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Nuša Verbič
Breda Novak
Lidija Živec (polovični delovni čas / part time)
Helena Radić (od septembra / from september)
Vesna Lenarčič (krajši delovni čas / part time)

ŠTUDENTI - PRAKTIKANTI / STUDENT PLACEMENTS (6 mes. / months)

Marjana Žnidar (od septembra / from september)
Barbara Ferenčak (od oktobra / from october)
Sabina Matjašec (od septembra / from september)



PODROČJA DEJAVNOSTI

Področje raziskovalne dejavnosti Laboratorija za analizno kemijo je analitika in kemijska karakterizacija materialov in procesov. Obsega študij in razvoj sodobnih analiznih metodologij in orodij za analizo (sledov) in določevanje kemijskih vrstnih elementov in spojin pri reševanju okoljskih, biomedicinskih, atmosferskih, industrijskih idr. problematik. Strokovna znanja in izkušnje članov Laboratorija za analizno kemijo so zelo široke in pokrivajo med drugim področja, kot so: elektrokemija (mikro-elektrode in senzorji), sklopljene tehnike (npr. tekočinska kromatografija in laserska ablacija v povezavi z ICP-masno spektrometrijo), ionska kromatografija, kemijski procesi v atmosferski vodni fazi, vzorčevanje in karakterizacija atmosferskih aerosolov (po velikostnih frakcijah), ICP-atomska emisijska spektrometrija, priprava vzorcev (razklop v mikrovalovni peči in sekvenčna/selektivna ekstrakcija) in modeliranje (ekstrakcijskih in separacijskih procesov). V naše raziskovalno delo so vključeni tudi podiplomski študenti, podoktorski gostje in specializanti. Dejavnost Laboratorija zajema tudi pogodbeno delo in storitve za neposredne industrijske in druge partnerje, kar vključuje razvoj in izboljšave metod ter analize vseh vrst vzorcev (okoljski, industrijski, biološki) in določevanje praktično vseh elementov periodnega sistema kot tudi

RESEARCH ACTIVITIES

The Analytical Chemistry Laboratory's field of research covers analytics, the chemical characterization of materials and processes and encompasses the study and development of modern analytical methodologies and tools for (trace) analysis and chemical speciation to solve selected problems in environmental, biomedical, atmospheric, industrial and related topics. The analytical expertise of the research team is very broad and covers amongst others electrochemistry (micro-electrodes and sensors), hyphenated techniques (such as liquid chromatography and laser ablation interfaced with ICP-Mass Spectrometry), ion chromatography, chemical processes in an atmospheric aqueous phase, sampling and characterization of size-segregated atmospheric aerosols, ICP-Atomic Emission Spectrometry, sample preparation (MW-assisted digestion and sequential/selective extraction) and modelling (extraction and separation processes).

The Analytical Chemistry Laboratory's activities also include contract work and special analytical services for industrial and other partners with emphasis on the development and adaptation of methods and analyses of all kind of samples (environmental, industrial, biological) and for determining practically all the elements in the periodic table, as well as many inorganic and organic ions.

mnogih anorganskih in organskih ionov ter drugih vrsti.

Več informacij na naši spletni strani
<http://www.ki.si/index.php?id=184>

BIBLIOGRAFIJA

- 11 izvirnih znanstvenih člankov
- 1 samostojni znanstveni sestavek v monografiji
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanja)
- 3 objavljeni znanstveni prispevki na konferencah
- 19 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 prispevek na konferenci brez natisa
- 1 vabljeni predavanja na konferenci brez natisa
- 2 končni poročili o rezultatih raziskav
- 6 elaboratov, predštudij, študij
- 1 diploma

GLAVNI DOSEŽKI V LETU 2006

- V sodelovanju s partnerjem iz Velike Britanije v okviru skupnega projekta smo okarakterizirali kemijske vrste arzena na odlagališču odpadkov iz procesa kalcinacije, pri čemer smo uporabljali vrsto različnih fizikalno-kemijskih metod, primernih za študij speciacije elementov, kot so XRD, XANES, EXAFS, sekvenčna ekstrakcija in sklopljene analizne tehnike. S kombinacijo omenjenih metod smo ugotovili, da je bil arzen prisoten predvsem v petvalentni obliki, vezan na amorfne in slabo kristalizirane okside železa (verjetno alfa-hematit). Našli smo tudi majhno količino neklasificirane kristalinične faze železovega arzenata. Kljub poprejšnjim drugačnim predpostavkam so celokupni rezultati te zahtevne raziskave torej pokazali, da je relativna "varnost" obravnavanih arzen vsebujočih odpadkov dokaj vprašljiva, saj je le majhen del arzena prisoten v kristalinični obliki kot nenevarni železov arzenat.
- Da bi pridobili boljši vpogled v okoljski cikel arzena, smo v okviru multilateralnega sodelo-

More information is available at: <http://www.ki.si/index.php?id=184&L=1>

BIBLIOGRAPHY

- 11 Original Scientific Articles
- 1 Independent Scientific Component Part in Monograph
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 3 Published Scientific Conference Contributions
- 19 Published Scientific Conference Contribution Abstracts
- 1 Unpublished Conference Contribution
- 1 Unpublished Invited Conference Lecture
- 2 Final Research Reports
- 6 Treatises, Preliminary Studies, Studies
- 1 Undergraduate Thesis

IMPORTANT ACHIEVEMENTS IN 2006

- In collaborative work with our partner from Great Britain, an array of physical-chemical techniques (XRD, XANES, EXAFS, Sequential Extraction Schemes and Hyphenated Elemental Speciation methods) were applied to characterize arsenic in a calciner residue dump (Cornwall, UK). Arsenic was predominantly present in pentavalent form, bound to amorphous or poorly-crystalline hydrous oxides of Fe (probably alpha-hematite). A small amount of a non-classified crystalline iron arsenate phase was found, viz. $\text{Fe}_2(\text{As}(\text{AsO}_4)_3)$. The overall results make us believe that the normally assumed relative safety, from a mobility point of view, is questionable since only a small fraction of arsenic is found in a crystalline iron arsenate form.
- In order to get a better understanding of the environmental cycling of arsenic and its chemical species, they were biomonitoring, within a multilateral cooperation study, in industrial areas in Portugal using transplanted lichens and tree bark. INAA, ICP-MS and HPLC-HGAFS were used to determine total arsenic and arsenic species. Since lichens contained methylated arsenic species, and aero-

vanja spremljali arzen in njegove spojine na industrijskih območjih Portugalske z uporabo biomonitoringa s transplantiranimi lišaji in drevesno skorjo. Za določitev celokupnih koncentracij arzena ter njegovih spojin smo uporabili INAA, ICP-MS in HPLC-HGAFS. Ker smo ugotovili, da so lišaji vsebovali metilirane arzenove spojine, atmosferski aerosoli z istih monitoring točk pa ne, smo sklepali, da se v tej študiji uporabljeni transplantirani lišaji ne obnašajo kot pasivni biomonitorji, ampak aktivno metilirajo arzen in ga transformirajo v biološko manj nevarno obliko.

- Sodelovali smo pri razvoju nove metode za določevanje železa (II) in celokupnega železa na osnovi sorpcije z uporabo SepPak C-18 kolone modificirane s ferozenom za določitev Fe(II), ali z 1-nitroso-2-naftolom za določitev celokupnega železa. V vrsti eksperimentov z radioaktivnimi sledilci smo preizkušali uporabnost metode za določanje zvrsti železa v morski vodi. Rezultati so pokazali, da je metoda primerna za določevanje zvrsti železa v morski vodi pri zelo nizkih koncentracijah (nmol/L).
- Rezultati študije, v okviru katere smo določili kemijsko sestavo in higroskopske lastnosti aerosolskih delcev po velikostnih razredih zbranih na slovenski obali, so pokazali, da je izvor zračnih mas pomemben faktor, ki vpliva na spremembe v kemijski sestavi glavnih komponent po velikostnih razredih. Razlika med dvema različnima izvoroma zračnih mas (kontinentalni in morski) se je najbolj odražala v koncentraciji vodotopnih organskih komponent v aerosolih, Cl^- , Na^+ , Mg^{2+} in Ca^{2+} , kakor tudi v faktorju povečanja mase aerosola z naraščajočo relativno vlago.
- V sodelovanju z avstrijskim partnerjem v okviru bilateralnega projekta smo izvedli primerjavo celokupnih koncentracij in masne porazdelitve ogljikovih ter drugih frakcij aerosolov po velikostnih razredih zbranih na dveh različnih urbanih lokacijah (Ljubljana in Dunaj, zimski čas). Kljub dokaj podobnim geografskim karakteristikam in vremenskim

sols from the same area did not, it could be concluded that the lichen transplants studied (*Parmelia caperata*) do not behave as genuine passive biomonitors but are able to actively methylate inorganic arsenic to methylated arsenic species.

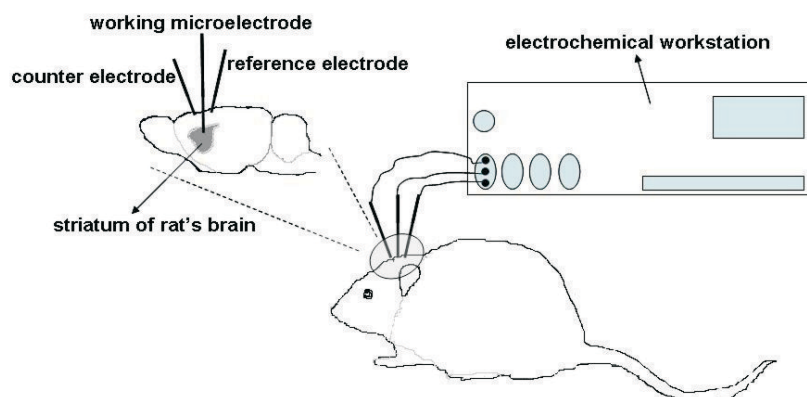
- We took part in a collaborative study on developing an approach to determine iron(II) and total iron, consisting of passing samples through preloaded SepPak C-18 cartridges with either ferrozine (FZ) for Fe(II) measurement or 1-nitroso-2-naphthol (1N2N) for the total iron analysis. A series of experiments was carried out to investigate the method's applicability for iron speciation in seawater using radio-iron. The described approaches were tested for seawater iron concentrations and are promising for iron speciation in the low nmol/L range.
- The results of a study on the chemical composition and water uptake characteristics of RHw size-segregated aerosols collected on the Slovenian coast showed that the origin of air masses is an important factor controlling the variation in the size distribution of the main components. The difference between the two different air mass origins (continental and marine) was particularly expressed for water soluble organic compounds, for Cl^- , Na^+ , Mg^{2+} and Ca^{2+} as well as in the mass growth factors of aerosols.
- In the framework of cooperation with our Austrian partner within a bilateral project we performed a comparison study on total concentrations and mass size distributions of carbonaceous and other fractions of aerosols collected at two different urban locations (Ljubljana and Vienna, during wintertime). Although the two sites seem rather similar (both for geographical characteristics and weather patterns in winter), there are some interesting differences. For example, the concentrations of low molecular weight carboxylic acids were much higher in Ljubljana (4 % vs. 1 % of the total mass), indicating different source characteristics for this fraction of

značilnostim so se pokazale nekatere zanimive razlike. Na primer: koncentracije nizkomolekularnih karboksilnih kislin so bile v Ljubljani bistveno višje (4 % vs. 1 % od celokupne mase), kar kaže na različen izvor. Druga pomembna razlika je bila v razmerju med BC (black carbon) in TC (total carbon), ki je za dunajske aerosole bistveno višje in kaže na višji prispevek dizelskih izpuhov.

- V okviru aplikativnega projekta smo izvedli druge, še obsežnejše meritve emisij delcev na dimniku Termo elektrarne Šoštanj. Specialni sistem za meritve emisij delcev po velikostnih razredih, ki smo ga razvili v našem laboratoriju, smo še dodatno nadgradili, tako da smo lahko vzorčevali tudi daljše čase. Vzoredno smo izpeljali tudi meritve emisij delcev po velikostnih razredih na dveh vplivnih lokacijah. Zbrane depozite delcev smo gravimetrično in kemijsko analizirali, pri čemer smo posebno pozornost posvetili potencialnim sledilcem iz tega izvora.
- Razvili smo metodologijo za hkratno direktno stripping voltametrično merjenje kobalta in niklja v nekaterih simuliranih in pravih

the aerosol. Another important difference is the BC/TC ratio (BC - black carbon, TC - total carbon), which was significantly higher for Vienna, indicating a larger contribution of diesel exhaust particles.

- In the framework of an applied research project we carried out an extensive campaign of aerosol emission measurements at the stack of a thermo-powerplant. A special system for the measurement of emission of size-segregated particles, designed in our lab, was additionally improved to allow the collecting of particles for a longer time. In parallel sampling, size-segregated particles were collected at two influential locations. All samples were then gravimetrically and chemically analyzed, with emphasis on determination of potential finger-prints for this source.
- We have developed a methodology for the use of a bismuth film microelectrode in the simultaneous direct stripping voltammetric measurement of trace cobalt and nickel in some simulated and real low-volume body fluids (tears, sweat, cerebrospinal fluid, aqueous humor). It has been demonstrated that



SLIKA 1:

Shematski prikaz in-vivo merjenja živčnih prenašalcev v možganih anestezirane eksperimentalne podgane z uporabo v našem laboratoriju razvitega elektro-kemijskega mikrosenzorja in ustrezne opreme (elektrokemijske delovne postaje).

FIGURE 1:

A schematic presentation of in-vivo measurement of neurotransmitters in the brain of an anesthetized experimental rat by application of an electrochemical microsensor, developed in our laboratory, and the appropriate instrumentation (electrochemical workstation).

nizkovolumskih vzorcih telesnih tekočin (solze, pot, cerebrospinalna tekočina, očesna vodica) z uporabo bizmutove tankoslojne mikroelektrode. Dokazali smo, da je to elektrodo možno uporabiti za določevanje obeh strupenih elementov v zelo majhnih vzorcih (100 do 400 mL) brez priprave vzorcev, razen razredčenja z ustreznim pufrom.

- Uporabo bizmutove tankoslojne elektrode (BiFE) smo razširili na merjenje kositra v povezavi z anodno stripping voltametrijjo. Pri tej novi metodi smo BiFE pripravili in-situ, t.j. sočasno z elektrolitsko predkoncentracijo s kateholom zakompleksanih kositrovih ionov. Ta elektroanalizna metoda z uporabo BiFE ima zelo dobre detekcijske karakteristike s spodnjo mejo zaznave 0,26 mg/L in je uporabna za določevanje kositra npr. v morski vodi.
 - Razvili smo tudi nov tip bizmutove elektrode, ki je osnovana na elektrodi iz ogljikove paste modificirani z bizmutovim prahom (Bi-CPE). Ta kompozitna elektroda združuje izjemne elektroanalizne karakteristike kovinskega bizmuta z vsemi prednostmi elektrod iz ogljikove paste. Po optimizirani sestavi kompozitnega elektrodnega materiala smo ugodne zmožljivosti Bi-CPE demonstrirali z anodnim stripping voltametrijjo nekaterih težkih kovin v sledovih, kot so Pb, Cd, Zn, Tl, In in Mn.
 - V sodelovanju s partnerji z Medicinske fakultete UL smo uspešno izvedli hkratno in-vivo merjenje treh pomembnih bioloških spojin dopamina, serotonina in askorbata v striatumu anesteziranih podgan (Sliki 1 in 2). Pri tem smo uporabili elektrokemijski mikrosenzor, ki je bil razvit v našem laboratoriju in temelji na elektrodi iz ogljikovega vlakna (premer 7 mm) prekrita z membrano iz preoksidiranega polifenilendiamina (OPPD/CFME). In-vivo meritve so pokazale izjemne lastnosti tega mikrosenzorja za detekcijo omenjenih spojin pod fiziološkimi pogoji, kar dokazuje, da ga je možno uporabljati pri pomembnih nevrofizioloških raziskavah.
- this modified microelectrode can be successfully applied to determine both toxic elements in microvolume samples (100 to 400 mL) without any sample pretreatment except for dilution with the appropriate buffer solution.
- The applicability of bismuth film electrodes (BiFE) has been expanded to the measurement of tin in combination with anodic stripping voltammetry. The BiFE was prepared in-situ, i.e. simultaneously with the electrolytic preconcentration of tin ions complexed with catechol. The electrode exhibited attractive electroanalytical performance, with a limit of detection of 0.26 mg/L, and can, for example be used for the measurement of tin in seawater.
 - In cooperation with our Czech partners we have developed a new type of bismuth electrode based on a carbon paste electrode modified with metallic bismuth powder (Bi-CPE). This composite electrode showed favourable synergistic characteristics for both components, the metallic bismuth and carbon paste. Upon the optimisation of the composite electrode material composition, the remarkable performance of Bi-CPE was demonstrated by applying anodic stripping voltammetric measurements of some trace heavy metals, such as Pb, Cd, Zn, Tl, In, and Mn.
 - In the framework of our collaboration with partners from a Medical School (ULJ) we have successfully carried out simultaneous in-vivo measurements of three significant biological compounds- dopamine, serotonin and ascorbate in the striatum of anesthetized rats (Figures 1 and 2). The experiments were performed using the microsensor (designed and prepared in our laboratory) based on a carbon fiber microelectrode (diameter of 7 mm) coated with a membrane of overoxidized poly-phenylenediamine. These in-vivo measurements demonstrated the applicability of the developed microsensor to simultaneously detect all three compounds under physiologi-

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V letu 2006 smo sodelovali z več deset industrijskimi in drugimi partnerji v okviru pogodb ali naročil za razvoj ali adaptacije in optimizacije metod oz. izdelave kemijskih analiz različnih vzorcev iz proizvodnje, okolja ali raziskav, ki zahtevajo posebna znanja in izkušnje ter specialno instrumentacijo; vse to nudimo v našem laboratoriju. Med najpomembnejše industrijske partnerje tovrstnega sodelovanja v letu 2006 sodijo:

- Salonit Anhovo d.d., Deskle;
- Lek d.d., Ljubljana;
- Belinka Perkemija d.o.o., Ljubljana;
- Pivovarna Union d.d., Ljubljana;
- Melamin d.d., Kočevje;
- Regeneracija d.o.o., Lesce;
- Eta d.o.o., Cerkno;
- Julon d.d., Ljubljana;
- Keko Varicon d.o.o., Žužemberk;
- Mitol d.d.; Sežana;
- Kolektor PRO d.o.o., Idrija;
- Tanin Sevnica;
- Pivovarna Laško d.d., Laško idr.

Sodelovanje z neindustrijskimi partnerji v letu 2006 je zajemalo pogodbeno in drugačno razvojno in raziskovalno delo z naslednjimi neposrednimi partnerji:

- Agencija Republike Slovenije za okolje, Ljubljana;
- Elektroinštitut Milan Vidmar, Ljubljana;
- Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani;
- Enota za patologijo prehrane in higieno okolja, NVI, Veterinarska fakulteta, Univerza v Ljubljani;
- Inštitut Jožef Stefan, Ljubljana;
- Fakulteta za strojništvo, Univerza v Mariboru;
- Zavod za gradbeništvo Slovenije, Ljubljana;
- Inštitut za hmeljarstvo in pivovarstvo Slovenije, Žalec;

cal conditions, making it promising for use in important neurophysiological studies.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

In 2006 we collaborated with several industrial and other partners within the framework of contracts and other types of cooperation for development and adaptation of methods and to perform analyses of various samples from industrial processes, the environment and research, all of which require the analytical expertise and special instrumentation that the Analytical Chemistry Laboratory can provide owing to its research activity.

A selected list of the most important industrial partners in 2006 comprises:

Salonit Anhovo d.d., Deskle; Lek d.d., Ljubljana; Belinka Perkemija d.o.o., Ljubljana; Pivovarna Union d.d., Ljubljana; Melamin d.d., Kočevje; Regeneracija d.o.o., Lesce; Eta d.o.o., Cerkno; Julon d.d., Ljubljana; Keko Varicon d.o.o., Žužemberk; Mitol d.d.; Sežana; Kolektor PRO d.o.o., Idrija; Tanin Sevnica; Pivovarna Laško d.d., Laško, all Slovenia etc.

Non-industrial partners for contract and research and development work in 2006 comprises:

Melamin d.d., Kočevje; Agency of the Republic of Slovenia for the Environment, Ljubljana; The "Milan Vidmar" Electroinstitute, Ljubljana; Faculty of Chemistry and Chemical Technology, University of Ljubljana; Unit for Pathology of Animal Nutrition and Environmental Hygiene (NVI, Veterinary Faculty, University of Ljubljana); Jožef Stefan Institute, Ljubljana; Slovenian Institute of Hop Research and Brewing, Agrochemistry department, Žalec; Faculty of Civil Engineering University of Maribor, Slovenian National Building and Civil Engineering Institute, Ljubljana; Laboratory for Astroparticle Physics and Laboratory for Environmental Research (Nova Gorica Polytechnic); Eye Clinic (Medical School, University of Ljubljana); Laboratory for Brain Research (Institute of Pathophysiology, Medical School, University of Ljubljana), all Slovenia etc.

- Laboratorij za astrofiziko osnovnih delcev in Laboratorij za raziskave v okolju, Univerza v Novi Gorici;
- Očesna klinika, Klinični center, Ljubljana;
- Laboratorij za raziskavo možganov, Inštitut za patološko fiziologijo, Medicinska fakulteta, Univerza v Ljubljani idr.

V letu 2006 smo nadaljevali z izvajanjem raziskovalno-aplikativnega projekta z naslovom: *Vpliv emisijskih virov na onesnaženje zraka s trdnimi delci* v sodelovanju z Elektroinštitutom Milan Vidmar in Termoelektrarno Šoštanj.

MEDNARODNO SODELOVANJE

V letu 2006 so bili sodelavci Laboratorija za analizo kemijo vključeni v naslednje mednarodne projekte:

- INTROP (Interdisciplinary Tropospheric Research: from the Laboratory to Global Change). Program evropske znanstvene fundacije; trajanje: 2004 – 2008; nacionalna koordinatorka in članica vodstvenega odbora: I. Grgič.
- COST Action 633 »Particulate Matter: Properties Related to Health Effects«, projekt poteka v okviru Evropske znanstvene fundacije; trajanje: 2002 – 2007; nacionalna koordinatorka ter podpredsednica COST 633: J. Turšič.
- Bilateralni projekt z naslovom: *Razvoj novih elektrokemijskih (mikro) senzorjev z uporabo sodobnih materialov za meritve v biomedicini in okoljevarstvu* (BI-US/06-07/22) v okviru slovensko-ameriškega znanstvenega sodelovanja; trajanje 2006 – 2007; partner: prof. Joseph Wang, Arizona State University; nosilec projekta: S. Hočevar.
- Bilateralni projekt z naslovom: *Možnosti analize z lasersko ablacijo – induktivno sklopljeno plazmo na področju konzervatorstva/restavriranja kulturne dediščine (steklo in keramika)* (BI-GB/06-021) v okviru slovensko-britanskega znanstvenega sodelovanja; partner: prof. Norman H. Tennent, Fyne Con-

In 2006, we continued carrying out the applied research project entitled "Influence of Emission on Ambient Air Pollution by Particulate Matter" in collaboration with the "Milan Vidmar" Electroinstitute, Ljubljana and the Thermopower plant Šoštanj, Slovenia.

INTERNATIONAL COLLABORATION

In 2006, the Analytical Chemistry Laboratory team members were involved in the following international projects:

- A European Science Foundation Program INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change"); duration: 2004 - 2008; national coordinator and member of the Steering Committee: I. Grgič.
- COST Action 633 project entitled "Particulate Matter: Properties Related to Health Effects" in the frame of European Science Foundation; duration: 2002 - 2007; national representative and vice-chair of COST 633: J. Turšič.
- A bilateral project entitled "Development of Novel Electrochemical (Micro)sensors Using Advanced Materials for Biomedical and Environmental Measurements" in the framework of S&T cooperation between Slovenia and the USA, 2006 – 2007. Partner: Prof. Joseph Wang, Arizona State University, USA. P.I.: S. Hočevar.
- A bilateral project entitled "Exploration of the Scope of Laser Ablation – Inductively Coupled Plasma Analysis in the Field of Conservation-Restoration of Cultural Heritage Comprising Glass and Ceramics" in the framework of S&T cooperation between Slovenia and Great Britain. Partner: Prof. Norman H. Tennent, Fyne Conservation services, St. Catherine's, Scotland, Great Britain. P.I.: J. T. van Elteren.
- A bilateral project entitled "Modelling of Separation Mechanisms in Modern Ion Chromatography: The Determination of Traces of Anions and Cations in Complicated Matrices and New Sample Preparation Tools and Meth-

servation Services, St. Catherine's, Scotland, UK; nosilec projekta: J. T. van Elteren.

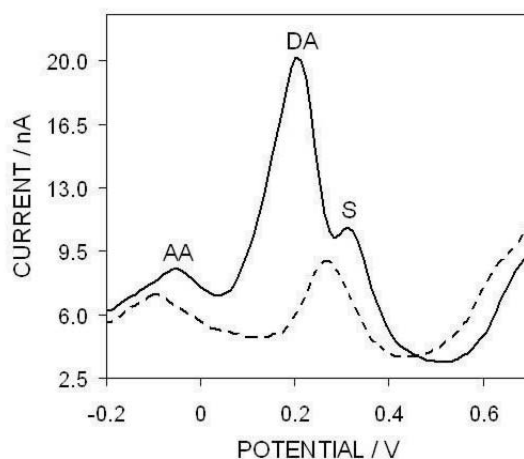
- Bilateralni projekt z naslovom: *Modeliranje separacijskih mehanizmov v moderni ionski kromatografiji: Določanje sledov anionov in kationov v kompleksnih vzorcih ter novi načini pred piprave vzorcev* (BI SLO-USA 07-07/29); partner: dr. Christopher Pohl, Dionex Corporation; nosilec projekta: Mi. Novič.
- Bilateralni projekt z naslovom *Nove aplikacije in matematično modeliranje separacijskih postopkov v ionski kromatografiji* (BI-CN/06-07/10); partner: prof. Zhu Yan, Zhejiang University, Department of Chemistry; nosilec projekta: Mi. Novič.

ods" in the framework of S&T cooperation between Slovenia and the USA. Partner: Ph.D. Cristopher Pohl, Dionex Corporation. P.I.: Mi. Novič.

- A bilateral project entitled "New Applications and Mathematical Modelling of Ion Chromatography Separation Procedures" in the framework of S&T cooperation between Slovenia and China. Partner: Prof. Zhu Yan, Zhejiang University, Department of Chemistry, China. PI: Mi. Novič.

MAJOR EQUIPMENT

- Inductively coupled plasma mass spectrometer (ICP-MS, Agilent Technologies, Model



SLIKA 2:

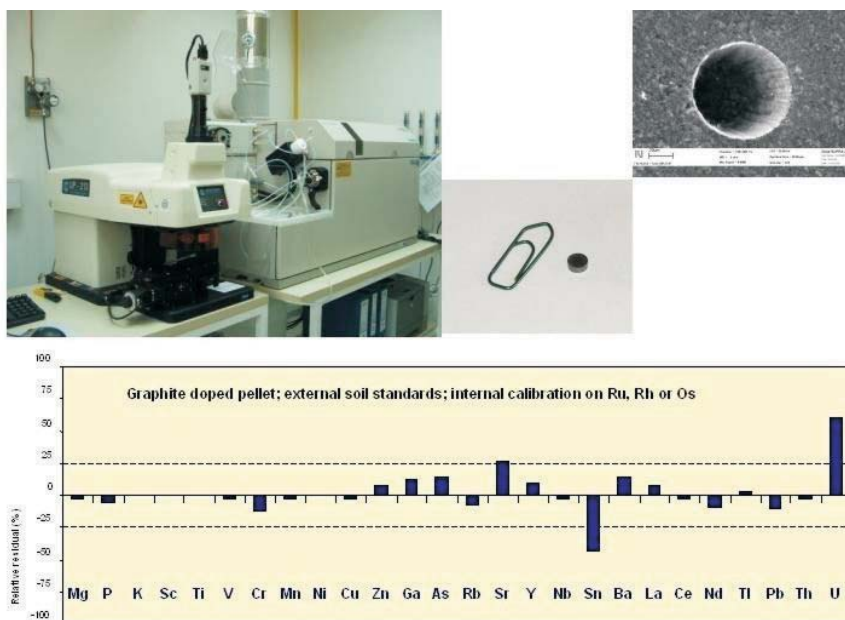
Voltametrična zapisa in-vivo meritev dopamina (DA), serotoninina (S) in askorbata (AA) z elektrokemijskim mikrosenzorjem v možganih (striatum) anestezirane poizkusne podgane po shemi, prikazani na sliki 1. Voltamogram označen s črtkano linijo predstavlja meritev izvedeno tik pred smrtjo, voltamogram označen s polno linijo pa meritev izvedeno ca. 90 s po nastopu smrti. Močno povečanje tokovno-napetostnega signala za živčni prenašalec dopamin takoj po smrti podgane je posledica kombinacije izločanja dopamina ob nastopu smrti in zmanjšane delovanja encima monoamino-oksidge ter prenehanja povratne regulacije nivoja dopamina.

FIGURE 2:

Voltammetric recordings of in-vivo measurements of dopamine (DA), serotonin (S) and ascorbate (AA) using an electrochemical microsensor in the brain (striatum) of an anesthetized experimental rat, according to the scheme displayed in Figure 1. The first voltammogram (dashed line) was recorded just prior to, and the second one (full line) approximately 90 s after the rat's death. A strong enhancement of the current response signal of the neurotransmitter dopamine is a consequence of a combination of continued dopamine secretion after death and a decreased activity of the monoamine-oxidase enzyme, as well as the termination of the reverse regulation of the dopamine level.

POMEMBNI INŠTRUMENTI IN OPREMA

- Masni spektrometer z induktivno sklopljeno plazmo (ICP-MS, Agilent Technologies, model 7500 ce&cs z dodatno opremo.
- Instrument za lasersko ablacijo, New Wave Research, model UP 213 A/F.
- Masni spektrometer z induktivno sklopljeno plazmo (ICP-MS, Hewlett Packard, model HP 4500 PLUS) s HPLC modulom in UV/Vis spektrometrom (DAD, Agilent, 1100 Series).
- 7500 ce&cs with additional accessories)
- Instrument for laser ablation (New Wave Research, Model UP 213 A/F)
- Inductively coupled plasma mass spectrometer (ICP-MS, Hewlett Packard, Model HP 4500 PLUS) with the HPLC module and diode array spectrophotometric detector (Agilent, 1100 Series)
- Inductively coupled plasma atomic emission spectrometer (ICP-AES, Thermo Jarrell Ash,



SLIKA 3:

Direktna multielementna analiza prsti (v obliki prešanega prahu) z uporabo sklopljenega analiznega sistema laserska ablacija - masni spektrometer z induktivno sklopljeno plazmo (LA-ICP-MS); grafitni prah, dopiran z Ru, Rh in Os kot internimi standardi, je služil kot vezivo pri pripravi tablete. Zgoraj levo: fotografija uporabljene LA-ICP-MS instrumentacije; zgoraj desno: tabletko s stisnjenim vzorcem prsti (sponka je priložena za primerjavo velikosti) in milroskopska slika ablacijskega kraterja (premer 80 μ m), ki ga je izdolbel laserski žarek; spodaj: rezultati analize vzorca standardnega materiala prsti prikazani v obliki odmikov od certificiranih vrednosti za koncentracije 26-tih merjenih elementov.

FIGURE 3:

Direct multi-elemental analysis of soil (in pressed powder form) using a hyphenated laser ablation – inductively coupled plasma mass spectrometer (LA-ICP-MS) system; graphite doped with Ru, Rh and Os is used as a binder with internal standardization properties. Top left: photo of the LA-ICP-MS instrumentation used; top right: pellet fabricated and a microscope image of an ablation crater

- Atomski emisijski spektrometer z induktivno sklopljeno plazmo (ICP-AES, Thermo Jarrell Ash, Model Atomscan 25) opremljen z ultrazvočnim razpršilcem (Cetac, model U-6000 AT).
- Vrstični elektronski mikroskop z visoko ločljivostjo (SEM) (Carl Zeiss, model SUPRA 35 VP) opremljen z energijsko disperzijskim spektrometrom (EDX) (Oxford Instruments, model Inca 400/SEM/EDX je skupna oprema več organizacijskih enot na inštitutu).
- UV/Vis spektrofotometer (Perkin Elmer, model Lambda 25).
- Sistem za ionsko kromatografijo (IC) s konduktometrično in spektrofotometrično detekcijo.
- Pretočno injekcijski analizator (ASIA Ismatec)
- Tri računalniško vodene elektrokemijske delovne postaje (Autolab, Eco Chemie) in en prenosni elektrokemijski sistem (PalmSens).
- Invertni optični mikroskop (Eclipse, Nikon).
- Oprema za izdelavo mikroelektrod (aparati za vlečenje kapilar, stereo leča, aparati za brušenje mikroelektrod, računalniško vodeni mikromanipulatori idr.).
- Reakcijska komora za raziskovanje reaktivnosti aerosolskih delcev pod kontroliranimi pogoji.
- Oprema za vzorčevanje aerosolov z Bernerjevimi nizkotlačnimi 10-stopenjskim kaskadnimi impaktorji.
- Mikrovalovna peč za razklope (MLS 1200 MEGA, Milestone).
- Sistem za pripravo čiste in ultračiste vode (Millipore) z Elix in Milli-Q Gradient enotama.
- Mikro in analize tehnice (Sartorius) nameščene v specialno klimatizirani tehtalnici (kontrola temperature in vlage) opremljeni z ionizatorjem.
- Model Atomscan 25) equipped with an ultrasonic nebulizer (Cetac, Model U-6000 AT)
- High resolution scanning electron microscope (SEM) (Carl Zeiss, model SUPRA 35 VP), equipped with an energy dispersive X-ray Spectrometer (EDX) (Oxford Instruments, model Inca 400) /SEM/EDX is shared with some other institute's research units
- UV/Vis spectrophotometer (Perkin Elmer, model Lambda 25)
- Ion chromatography (IC) system with conductivity and spectrophotometric detection
- Flow injection analyzer (ASIA Ismatec)
- Three computer assisted electrochemical workstations (Autolab, Eco Chemie) and a portable electrochemical system (PalmSens)
- Inverted optical microscope (Eclipse, Nikon)
- Microelectrode fabrication tools (capillary puller, stereo-zoom microscope, microelectrode beveller, computerised micromanipulator, etc.)
- Reaction chamber for the investigation of aerosol particle reactivity under controlled conditions
- Equipment for aerosol sampling (low-pressure Berner-type cascade impactors)
- Microwave oven for sample digestion (MLS 1200 MEGA, Milestone)
- Micro and analytical balances (Sartorius) placed in a specialised air conditioned (temperature and humidity control) room equipped with an ion emitter
- Water purification system (Millipore) including Elix and Milli-Q Gradient units

EDUCATION AND IMPORTANT VISITS

Visits abroad:

- J.T. van Elteren, 6-week research visit to Prof. P. R. D. Mason, Utrecht University, The Netherlands.
- L. Mauko, 3-week study visit to Prof. K. Kalcher, Institute of Chemistry, Karl-Franzens University, Graz, Austria.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Obiski v tujino:

- J.T. van Elteren je bil na 6-tedenskem delovnem obisku pri prof. P. R. D. Masonu na Utrecht University, Nizozemska.
- L. Mauko je bila na 3-tedenskem izpopolnjevanju pri prof. K. Kalcherju na Institute of Chemistry, Karl-Franzens University, Graz, Avstrija.
- J.T. van Elteren je bil na enotedenskem delovnem obisku pri prof. N. H. Tennantu v Fine Conservation Services, Glasgow, Velika Britanija.
- J.T. van Elteren je bil na enotedenskem delovnem obisku pri prof. A.C. Cefalasu na Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Atene, Grčija.
- Mi. Novič je bil na 10-dnevem delovnem obisku v Dionex, Sunnyvale, CA, ZDA.
- S. Hočevar je bil na 8-dnevem delovnem obisku pri prof. S. Danieleju na University of Venice, Benetke, Italija.
- S. Hočevar je bil na 3-tedenskem delovnem obisku pri prof. J. Wangu na Center for Bioelectronics and Biosensors, Arizona State University, Tempe, AZ, ZDA.

Obiski iz tujine:

- Michael Beeston z University of Exeter (Velika Britanija) je bil na več mesečnem delovnem obisku in je pod vodstvom somentorja dr. van Elterena opravljaval raziskovalno delo za doktorsko disertacijo.
- Prof. N. H. Tennant s Fine Conservation Services, Glasgow, Velika Britanija, je bil na enotedenskem delovnem obisku v okviru bilateralnega projekta.
- Doc. dr. Valentin Mirčeski z Univerze v Skopju, Makedonija, je bil na 3-dnevem delovnem obisku.

- J.T. van Elteren, one-week research visit to Prof. N. H. Tennant, Fine Conservation Services, Glasgow, Scotland.
- J.T. van Elteren, one-week research visit to Prof. A. C. Cefalas, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece.
- Mi. Novič, 10-day research visit to Dionex, Sunnyvale, CA, USA.
- S. Hočeva, 8-day research visit to Prof. S. Daniele, University of Venice, Venice, Italy.
- S. Hočevar, 3-week research visit to Prof. J. Wang, Center for Bioelectronics and Biosensors, Arizona State University, Tempe, AZ, USA.

Visits from abroad:

- Mr. Michael P. Beeston from the University of Exeter, Great Britain, has been on a several month work visit under the supervision of his co-mentor, Dr. van Elteren from our laboratory to perform part of his Ph.D. research program.
- Prof. N. H. Tennant, Fine Conservation Services, Glasgow, Scotland, one-week visit in the framework of a bilateral project.
- Prof. Valentin Mirčeski University of Skopje, Macedonia, three-day work visit.

L05

Laboratorij za kemijo,
biologijo in tehnologijo vod

Laboratory for Chemistry,
Biology and Technology of Water



VODJA / HEAD
Prof. dr. Milenko Roš

RAZISKOVALCI / RESEARCHERS

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doc. dr. Andreja Drolc
doc. dr. Tatjana Tišler
dr. Janez Vrtovšek
prof. dr. Jana Zagorc Končan
dr. Gregor D. Zupančič

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Anita Jemec
Tanja Kurbus

TEHNIČNO OSEBJE / TECHNICAL STAFF

Jelka Jelnikar
Emil Meden
Matjaž Omerzel

PRIPRAVNIKI / TRAINEES

Carolina Miranda Ribeiro (IAESTE)
Jan Zupančič (1 mesečna dijaška praksa / 1 month)
Kristina Krajnc (6 mesečna študentska praksa / 6 months)
Petra Igljučar (3 mesečna študentska praksa / 3 months)



PODROČJA DEJAVNOSTI

- a) Raziskovalni program:
- Integralni pristop k preprečevanju onesnaževanja voda (Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani); nosilec: M. Roš.
- b) Raziskovalni in razvojni projekti:
- Meroslovna sledljivost v kemiji – vloga referenčnih materialov in referenčnih merjenj (Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani); nosilka: A. Drolc;
 - Razvoj postopka za stabilizacijo, mineralizacijo in higienizacijo blata iz malih čistilnih naprav (Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani, Komunarno podjetje Velenje); nosilec: G. D. Zupančič;
 - Kemijsko in biološko sledenje ne nukleotidov in njihovega vpliva v okolju (Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani); nosilka: P. Trebše, Politehnika Nova Gorica;
 - Biološki testi za ugotavljanje toksičnosti in

RESEARCH ACTIVITIES

- a) Research programme
- Integrated Approach to Water Pollution Prevention (Ministry of Higher Education, Science and Technology, Republic of Slovenia) – Principal investigator: M. Roš
- b) Research and applied projects:
- Metrological Traceability in Chemistry – Role of Reference Materials and Reference Measurements (Ministry of Higher Education, Science and Technology, Republic of Slovenia) – Principal investigator: A. Drolc;
 - Procedure Development for Stabilization, Mineralization and Hygienization of Wastewater Sludge from Small WWTP (Ministry of Higher Education, Science and Technology, Republic of Slovenia, Municipality of Velenje) – Principal investigator: G. D. Zupančič;
 - Chemical and Biological Monitoring of Neonicotinoids and Their Impact Assessment in the Environment (Ministry of Higher Education, Science and Technology, Republic of Slovenia) - Principal researcher: Dr.

- genotoksičnosti vode, zemlje in hrane (Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani); nosilka: R. Marinšek Logar, Biotehniška fakulteta;
- Razvoj celovitega sistema za ugotavljanje toksičnosti in genotoksičnosti v zemlji, vodi in hrani v soglasju s smernicami Evropske unije (Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani); nosilka: R. Marinšek Logar, Biotehniška fakulteta;
 - Preučevanje škodljivih učinkov in mehanizmov dolgotrajnega delovanja organofosfornih snovi na ljudi, živali in okolje in načrtovanje ustreznih protiukrepov; vodja projekta: Matjaž Harmel, Oikos, Domžale;
 - Organiziranje medlaboratorijskih primerjav za laboratorije, ki izvajajo monitoring odpadnih vod (Ministrstvo za okolje in prostor, Agencija RS za okolje);
 - Zagotavljanje sledljivosti (Urad Republike Slovenije za meroslovje);
 - Pridobivanje obnovljive energije iz organskih substratov (Pivovarna Union, Ljubljana; Lek d.d., Ljubljana).
- d) Center odličnosti – okoljske tehnologije
Sodelovanje na projektih:
- Razvoj novih metod za čiščenje odpadnih vod v SBR;
 - Biološka stabilizacija blata.
- e) Vzdrževanje sistema kakovosti v skladu s standardom SIST EN ISO/IEC 17025.

BIBLIOGRAFIJA

- 3 izvorni znanstveni članki
- 2 poljudna članka
- 1 drugi članek ali sestavek
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanje)
- 1 objavljeni strokovni prispevek na konferenci (vabljeni predavanje)
- 15 objavljenih znanstvenih prispevkov na konferencah
- 4 objavljeni strokovni prispevki na konferencah

- Polonca Trebše (University of Nova Gorica);
 - Biological Tests for Toxicity and Genotoxicity Determination in Water, Soil, and Food (Ministry of Higher Education, Science and Technology, Republic of Slovenia) - Principal researcher: Prof. Dr. Romana Marinšek Logar (Biotechnical faculty, University of Ljubljana);
 - Development of an integrated system for assessment of toxicity and genotoxicity in soil, water and food in concordance with the EU directives (Ministry of Higher Education, Science and Technology, Republic of Slovenia) - Principal researcher: Prof. Dr. Romana Marinšek Logar (Biotechnical faculty, University of Ljubljana);
 - Study of harmful effects and mechanisms of long term exposures of organophosphorus compounds to human, animals and environment and plans for corresponding preventive measures, Principal researcher: Matjaž Harmel, Oikos, Domžale, Slovenia;
 - Organization of Interlaboratory Comparisons for Slovenian Laboratories which Perform Monitoring of Waste Water (Agency for the Environment);
 - Renewable Energy – Biogas Production from Various Organic Substrates (Union Brewery, Ljubljana, Slovenia, pharmaceutical substrate – Lek d.d., Ljubljana, Slovenia).
- d) EU Centre of excellence – environmental technologies
- Participation on projects:
 - Development of waste water treatment procedures in SBR
 - Biological sludge treatment
- e) Operation of laboratory according to requirements of the standard SIST EN ISO/IEC 17025

BIBLIOGRAPHY

- 3 Original Scientific Articles
- 2 Popular Articles
- 1 Other Article or Component Part
- 1 Published Scientific Conference Contribution (Invited Lecture)

- 12 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 3 prispevki na konferencah brez natisa
- 7 vabljenih predavanj na konferenci brez natisa
- 8 končnih poročil o rezultatih raziskav
- 6 elaboratov, predštudij, študij
- 4 diplome
- 2 magisterija

GLAVNI DOSEŽKI V LETU 2006

- Preučevali smo kinetiko procesov biološkega čiščenja v dveh šaržnih reaktorjih pri visoki starosti oziroma koncentraciji biomase ($X > 10$ g/L). Prvi reaktor je deloval s klasično tehnologijo z dispergirano biomaso, v drugem pa smo uvajali novo tehnologijo čiščenja z granulirano biomaso. V obeh reaktorjih smo dosegli visoko učinkovitost čiščenja ob odličnih usedalnih lastnostih blata.
- Izvedli smo tudi prve preskuse na področju separacije mikroorganizmov z membranami (filtri). Kot filter smo uporabili material, katerega delovanje ne temelji na velikosti por, temveč na lastnostih nano delcev dodanega anorganskega materiala. Ti preskusi bodo služili kot osnova za študij na področju membranskih bioreaktorjev (MBR).
- Razvili smo nov proces za namen pridobivanja bioenergije: anaerobne obdelave odpadnih gošč in močno obremenjenih voda, kjer obremenitev reaktorja lahko 2,5 krat preseže obremenitev običajnega procesa.
- Razvili smo aerobno tehnologijo obdelave blata za majhne čistilne naprave. Proces je prirejen za ČN do 5000 PE. Uporabili smo autotermalni efekt za doseglo higienizacije blata, pri tem pa smo precej povečali učinek odstranitve organskih komponent in hraniv, kot je amonijev dušik.
- Določili smo tehnologijo običajne anaerobne soobdelave izčrpanega odvečnega micelija iz proizvodnje farmacevtskih učinkovin z drugimi običajnimi substrati do te mere, da

- 1 Published Professional Conference Contribution (Invited Lecture)
- 15 Published Scientific Conference Contributions
- 4 Published Professional Conference Contributions
- 12 Published Scientific Conference Contribution Abstracts
- 3 Unpublished Conference Contributions
- 7 Unpublished Invited Lectures at a Conference
- 8 Final Research Reports
- 6 Treatises, Preliminary Studies, Studies
- 4 Undergraduate Theses
- 2 Master's Theses

IMPORTANT ACHIEVEMENTS IN 2006

- Biological treatment processes were studied in two Sequencing Batch Reactors (SBRs). In the first SBR (anoxic/aerobic) high flocculent biomass concentration ($X > 10$ g/L) was achieved with long solid retention time (SRT). In the second SBR (aerobic) high biomass concentration ($X > 10$ g/L) was achieved with granulation. High treatment efficiency and good biomass settling properties were realised in both SBRs.
- Basic microfiltration tests with nano material membranes were performed for the introduction of the Membrane BioReactor (MBR) technology.
- We developed the technology for the anaerobic treatment of organic waste and slurries. The process is designed to sustain 2.5 times higher organic loads than conventional processes.
- We developed an aerobic treatment of waste sludge from small WWTP's. The technology is suitable for WWTP's up to 5000 PE. We used auto-thermal properties to achieve pathogen removal and at the same time managed to substantially increase volatile solids removal and nitrogen ammonia removal as well.

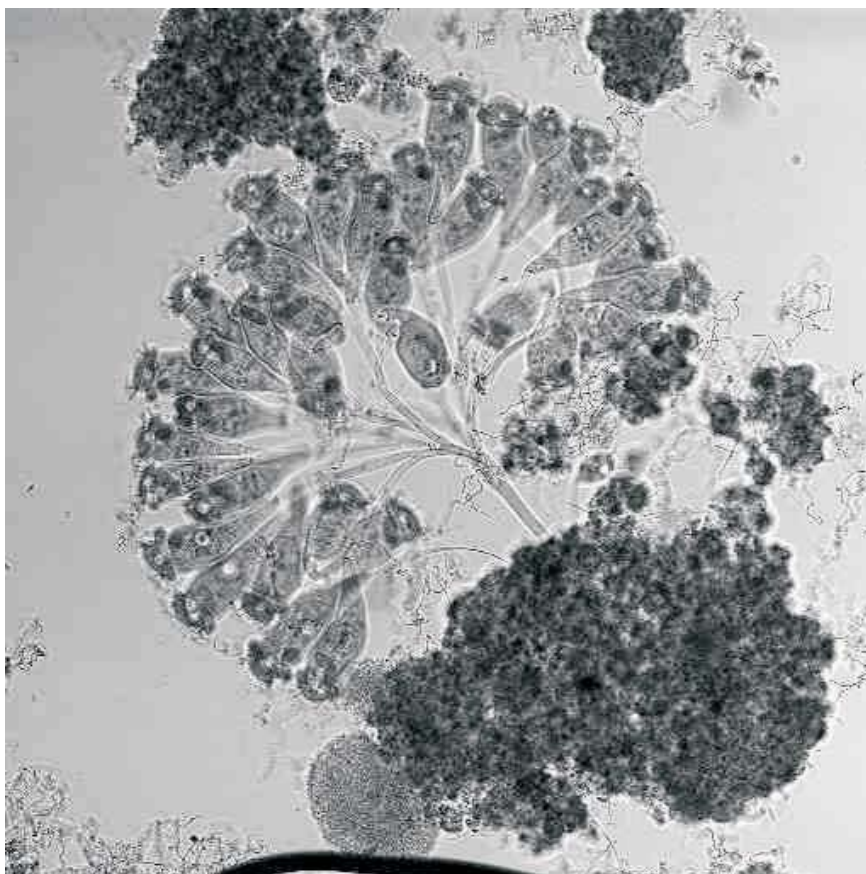
- je proces pridobivanja bioplina nemoten in da ostanek obdelave ni škodljiv okolju.
- Razvili smo metode za določanje subletalnih vplivov strupenih snovi na aktivnosti biokemijskih biomarkerjev v rakih vodne bolhe (*Daphnia magna*), ki nam omogočajo zaznavanje sprememb že pri nizkih koncentracijah strupenih snovi v vodi. Vodne bolhe smo za 21 dni izpostavili kromu, kadmiju in različnim pesticidom ter ugotavljali preživetje in razmnoževanje vodnih bolh ter določili aktivnosti acetilholinesteraze, glutation S-transferaze in katalaze.
 - Uvedli smo biološki preskus za določanje prisotnosti estrogenov in drugih ksenoestrogenih motilcev hormonskega sistema v odpadnih vodah s kvasovko *Saccharomyces cerevisiae*.
 - Nadaljevali smo tudi z optimizacijo ATP metode za določanje strupenosti dotokov na biološke čistilne naprave v smislu primerjave občutljivosti z že uveljavljenima testoma strupenosti z bakterijami *Vibrio fischeri* in mikroorganizmi aktivnega blata.
 - We also developed the technology for the conventional anaerobic treatment of waste mycelia from pharmaceutical industry production combined with other common organic substrates. We managed to sustain and increase biogas production from mycelia as well as to produce treatment residue, which can be used as fertilizer without adverse effects to environment.
 - We developed the methods for determining sub lethal effects of pollutants on the activity of biochemical biomarkers in the water flea *Daphnia magna* with the aim to detect early changes at cellular levels in aquatic organisms at low toxic concentrations of chemicals. Methods for measuring the activity of biochemical biomarkers were optimised after long term, chronic exposure to toxic chemicals. During 21 days of exposure to chromium, cadmium and pesticides the survival and reproduction of water fleas was checked and the activity of acetyl cholinesterase, glutathione S-transferase and catalase were determined.



SLIKA 1:
čistilna naprava Javor Furnir, Prestranek

FIGURE 1:
Industrial wastewater treatment plant Javor Furnir, Prestranek

- Na področju meroslovja v kemiji smo razvili metodologijo za pripravo referenčnih materialov za izbrane merjene veličine ob upoštevanju vseh značilnosti, ki bi lahko vplivale na integriteto testnih vzorcev, predvsem homogenost in stabilnost vzorcev. Pripisane vrednosti merjenih veličin referenčnih materialov, ki smo jih uporabili pri izvedbi medlaboratorijske primerjave, smo določili na osnovi referenčnih merjenj. Referenčna merjenja smo izvajali na osnovi validiranih metod, pri čemer so bili rezultati merjenj sledljivi do mednarodnih referenc z ocenjeno merilno negotovostjo. Uspešnost sodelovanja laboratorijev smo ovrednotili z izračunom Z-rezultata.
- A bioassay with modified yeast *Saccharomyces cerevisiae* which contain human receptor in genome was introduced to detect estrogens and xenoestrogens in waste waters.
- Sensitivity of the ATP method proposed for toxicity measurement of inflows into biological waste water treatment plants was compared with standardised methods using bacteria *Vibrio fischeri* and micro-organisms of activated sludge.
- In the field of metrology in chemistry a methodology for the preparation of reference materials for selected measurands was developed. All the indications that could affect the integrity of test samples, such as stability



SLIKA 2:
Organizmi v aktivnem blatu iz SBR – povečava-10×

FIGURE 2:
Organisms in the activated sludge from SBR – magnification-10×

- Uspešno smo predstavili sistem kakovosti Laboratorija za kemijo, biologijo in tehnologijo vod na konferenci EUROMET – tehnični odbor Kakovost, Malta, februar 2006.
- Izvedli smo dve medlaboratorijski primerjavi za slovenske in tuje laboratorije, ki izvajajo monitoring odpadnih vod in mednarodno delavnico na področju meroslovja v kemiji, skupaj z JRC-IRMM, Belgija.
- Bili smo vpisani v mednarodno bazo EPTIS (BAM Nemčija), kot prva in edina slovenska shema medlaboratorijskih primerjav.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Biotehniška fakulteta: Oddelek za biologijo in Oddelek za zootehniko, Univerza v Ljubljani;
- Dr. Duhovnik d.o.o., Seničica;
- Esotech d.d., Velenje;
- Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani;
- Geološki zavod Slovenije, Ljubljana;
- Inštitut za fizikalno biologijo, Grosuplje;
- Komunalna Energetika Ljubljana (KEL), Ljubljana;
- Komunalno Podjetje Velenje d.o.o., Velenje;
- LEK d.d., Ljubljana;
- Ministrstvo za okolje in prostor – Agencija RS za okolje, Ljubljana;
- Nuklearna elektrarna Krško, Krško;
- Oikos, Svetovanje za razvoj, Domžale;
- Pivovarna Union, Ljubljana;
- Univerza v Novi Gorici, Nova Gorica;
- Urad Republike Slovenije za meroslovje, Ljubljana;
- Veterinarska fakulteta, Univerza v Ljubljani;
- Zavod za gradbeništvo Slovenije (ZAG), Ljubljana.

and homogeneity were taken into account. Reference values of the test material, which are the base for evaluating results, were determined using reference measurements. Reference measurements were performed using validated methods – results were traceable to international references and measurement uncertainty of the results was evaluated. The laboratory's performance was evaluated by calculating Z-score.

- The quality system of the Laboratory for Chemistry, Biology and Technology of Water was successfully presented at EUROMET conference – TC Quality, in February 2006 in Malta.
- We provided two distributions of samples in the ILC-Waste Water and organized an international workshop together with JRC-IRMM Belgium.
- The ILC-Waste Water is registered in the EPTIS database.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Biotechnical Faculty: Departments for Biology and Zootechnic, University of Ljubljana, Slovenia;
- Dr. Duhovnik d.o.o., Seničica, Slovenia;
- Esotech d.d., Velenje, Slovenia;
- Faculty for Chemistry and Chemical Technology, University of Ljubljana, Slovenia;
- Geological Survey of Slovenia, Ljubljana, Slovenia;
- Institute for Physical Biology, Grosuplje, Slovenia;
- Public Utility Energetics, Ljubljana, Slovenia;
- Municipality of Velenje, Velenje, Slovenia;
- LEK - Sandoz Company, Ljubljana, Slovenia;
- Ministry of Environment and Spatial planning
- Environmental Agency, Republic of Slovenia;
- Nuclear Power Plant Krško, Krško, Slovenia;
- Oikos, Development Consulting, Domžale, Slovenia;

MEDNARODNO SODELOVANJE

- European Analytical Quality Control via Water Information System for Europe (EAQC-WISE), 6. OP, 2005-2008, pogodba št. 022603
- Training in Metrology in Chemistry (TrainMiC)

POMEMBNI INŠTRUMENTI IN OPREMA

- Anaerobni reaktor z opremo,
- anaerobni SBR reaktor,
- ATAD-SBR reaktor,
- avtomatizirani respirometer (MICRO-Oxymax 6.0, Columbus Instruments),
- avtomatizirani šaržni biološki reaktor (ŠBR),
- čitalec mikrotiterskih plošč (Bio-tek, Micro-Wave XS),

- Union Brewery, Ljubljana, Slovenia;
- University of Nova Gorica, Faculty for Environmental Sciences, Nova Gorica, Slovenia;
- Metrology Institute of the Republic of Slovenia;
- Veterinary faculty, University of Ljubljana, Slovenia;
- Slovenian National Building and Civil Engineering Institute, Ljubljana.

INTERNATIONAL COLLABORATION

- European Analytical Quality Control via Water Information System for Europe (EAQC-WISE), 6. FP, 2005-2008, Contract no. 022603;
- Training in Metrology in Chemistry (TrainMiC).



SLIKA 3:

Odločba o priznanju etalona v okviru nacionalnega etalona za množino snovi

FIGURE 3:

Designation of holder of the national standard in the frame of national standard for the unit amount of substance

- ionski kromatograf (DIONEX 120) s samodejnim vzorčevalnikom,
- Kjeltec sistem 2300 Autosystem II (FOSS Tecator) za razklop in določanje Kjeldahlovega dušika,
- kombinirani anaerobno-anoksičnoaerobni reaktorji (KI),
- laboratorijski modeli bioloških čistilnih naprav,
- laboratorijski modeli rek,
- LUMIS-TOX aparatura (dr. Lange),
- spektrofotometer Lambda 20 (Perkin-Elmer) Agilent Technologies 6890 N GC System + 5973 Mass selective Detector,
- TOC analizator TOC-5000A (SHIMADZU).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Izobraževanje:

- Doc. dr. Andreja Drolc je habilitirana na področju varstva okolja in predava predmet Onesnaževanje zraka, vode in tal (Univerza v Novi Gorici);
- prof. dr. Milenko Roš je habilitiran za področje onesnaževanje in zaščita voda in predava predmet Zaščita voda (Univerza v Novi Gorici);
- doc. dr. Tatjana Tišler je habilitirana za področje toksikologije in predava predmet Ekotoksikologija (Univerza v Novi Gorici).

Obiski in gostovanja:

- Priprava modula "Sampling" v okviru TrainMiC (Training in Metrology in Chemistry) projekta, na Inštitutu za referenčne materiale in merjenja, Geel, Belgija (JRC-IRMM) (M. Roš);
- mentorstvo in somentorstvo ter delovno mentorstvo diplomskih, magistrskih in doktorskih del (M. Cotman, A. Drolc, M. Roš, T. Tišler, J. Vrtovšek, J. Zagorc-Končan, G. Zupančič);
- soorganizacija delavnice TraiMiC, skupaj z JRC-IRMM, Geel, Belgija (M. Roš, M. Cotman, A. Drolc),
- soorganizacija konference z mednarodno udeležbo, VODNI DNEVI 2006, kjer so

MAJOR EQUIPMENT

- Anaerobic reactor with equipment;
- Anaerobic SBR reactor;
- ATAD-SBR reactor;
- Automated respirometer (MICRO-Oxymax 6.0, Columbus Instruments);
- Automated sequencing Batch Reactor (SBR);
- Micro-plate reader (Bio-tek, Micro-Wave XS);
- Ion chromatograph (DIONEX 120) with automated sampler (DIONEX);
- Kjeltec system 2300 Auto system II (FOSS Tecator) for Kjeldahl N determination;
- Combined anaerobic-anoxic reactors;
- Laboratory wastewater treatment plants;
- Laboratory river models;
- LUMIS-TOX apparatus (dr. Lange);
- Spectrophotometer Lambda 20 (Perkin-Elmer) ;
- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector;
- TOC analyser TOC-5000A (SHIMADZU).

EDUCATION AND IMPORTANT VISITS

Education:

- Dr. Andreja Drolc, Assist. Prof., is qualified as a university teacher for the field *Environmental Protection*; she lectures on the subject of *Air, Water and Soil Pollution* (University of Nova Gorica, Slovenia);
- Prof. Dr. Milenko Roš is qualified as a university teacher for the field of *Water Pollution and Protection*; he lectures the subject of *Water Protection* (University of Nova Gorica, Slovenia);
- Dr. Tatjana Tišler, Assist. Prof., is qualified as a university teacher in the field of *Toxicology*; she lectures the subject *Ecotoxicology* (University of Nova Gorica, Slovenia).

Important visits:

- Preparation of the module "Sampling" module in the frame of TrainMiC (Training of Measurements in Chemistry) project, at the

sodelavci laboratorija sodelovali kot predavatelji;

- udeležba na AQUAbase workshop: Risk assessment of organic micro pollutants in the aquatic environment, Aachen, Nemčija; 28. – 29. 11. 2006 (T. Tišler, A. Jemec);
- strokovna praksa v organizaciji IAESTE Ljubljana (Carolina Miranda Ribeiro);
- udeležba in predavanje na TrainMiC Jambooree, Geel, Belgija, 16. – 21. junij 2006 (M. Roš in A. Drolc).

Kemijski inštitut, Laboratorij za kemijo, biologijo in tehnologijo vod je bil februarja 2006 s strani Urada RS za meroslovje imenovan za *nosilca etalona v okviru nacionalnega etalona enote množina snovi* (področje: varovanja okolja, vrsta vzorca: odpadne in površinske vode).

Institute for Reference Materials and Measurements, Geel, Belgium (JRC-IRMM) (M. Roš).

- Mentorship for diploma, masters and doctoral theses (M. Cotman, A. Drolc, M. Roš, T. Tišler, J. Vrtovšek, J. Zagorc-Končan, G. Zupančič).
- Co-organisation of TrainMiC workshop, with JRC-IRMM, Geel, Belgium (M. Roš, M. Cotman, A. Drolc).
- Co-organisation of the conference as well as international participation, Water Days 2006, co-workers of the Laboratory were also lecturers.
- Participation at AQUAbase workshop: Risk Assessment of Organic Micro Pollutants in the Aquatic Environment, Aachen, Germany; November 28 – 29, 2006 (T. Tišler, A. Jemec)
- Technical practice for IAESTE Ljubljana (Carolina Miranda Ribeiro)
- Participation and lecture at TrainMiC Jambooree, Geel, Belgium, June 16 – 21, 2006 (M. Roš and A. Drolc)

National Institute of Chemistry, Laboratory for Chemistry, Biology and Technology of Water have been designated by the Metrology Institute of the Republic of Slovenia as *the holder of national standard in the frame of national standard for amount of substance* (area: Environmental protection, sample: wastewater and surface water)

L06

Laboratorij za prehrambeno kemijo

Laboratory for Food Chemistry



VODJA / HEAD
Dr. Mirko Prošek

RAZISKOVALCI / RESEARCHERS

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Dr. Andrej Šmidovnik
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**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Maja Fir
Vesna Glavnik
Mitja Križman
Mitja Martelanc
Kajetan Trošt

TEHNIČNO OSEBJE / TECHNICAL STAFF

Mateja Puklavc

PRIPRAVNIKI / TRAINEES

Barbara Kapun



PODROČJA DEJAVNOSTI

Raziskovalno delo v Laboratoriju za prehrabeno kemijo (L06) je usmerjeno na področje razvoja prehranskih dodatkov in vrednotenja spojin naravnega izvora. Delo poteka v petih podskupinah, in sicer:

- na razvoju novih prehrabnih izdelkov in prehranskih dodatkov s funkcionalnimi lastnostmi;
- na pripravi in vrednotenju specialne prehrane in na prehrabnem inženiringu;
- na določanju spojin naravnega izvora s sodobnimi kromatografskimi in spektroskopskimi tehnikami;
- na razvoju in validaciji novih analiznih metod in analiznih tehnik;
- na preprečevanju kemijskih tveganj z upoštevanjem dobrih praks (GLP in GMP) pri razvoju in validaciji analiznih metod, tehnološke validacije, validacije čiščenja in HCCAP-a.

RESEARCH ACTIVITIES

Research activities are oriented toward scientifically designed food for healthy nutrition. They are divided into five main fields:

- Development of new food products and food additives with functional activities
- Evaluation of special food and food engineering
- Investigation of compounds from natural sources by modern chromatographic and spectroscopic techniques
- Development and validation of new analytical techniques and methods
- Minimization of chemical hazards in food production according to GLP, GMP and HCCAP

BIBLIOGRAPHY

- 7 Original Scientific Articles
- 1 Published Scientific Conference Contribution
- 18 Published Scientific Conference Contribution Abstracts
- 1 Patent Application

BIBLIOGRAFIJA

- 7 izvirnih znanstvenih člankov
- 1 objavljeni znanstveni prispevek na konferenci
- 18 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 patentna prijava
- 1 patent
- 3 diplome

GLAVNI DOSEŽKI V LETU 2006

Raziskave so potekale na področju prehrabene in analize kemije in v sodelovanju z zunanjimi partnerji pri razvoju novih prehrabnih dodatkov in živil obogatenih s koencimom Q10. Razvojno raziskovalne naloge so bile vezane na razvoj, optimizacijo, validacijo in uporabo raznih analiznih tehnik in metod. Pri vrednotenju prehrabnih in farmacevtskih izdelkov, kakor tudi pri zasledovanju aktivnih komponent v bioloških poizkusih, smo uspešno uporabljali separacijske in spektroskopske tehnike in njihove povezave.

V sodelovanju z zunanjimi raziskovalnimi institucijami in v sklopu lastnih projektov smo pripravili metode za vrednotenje učinkovin rastlinskega in živalskega izvora, ki so pomembne za človekovo zdravje. Skupaj z Veterinarsko fakulteto smo razvili nove metode za kvantitativno vrednotenje sladkorjev v plazmi z masno spektrometrijo in s to metodo pri psih ugotavljali poškodovanost črevesne sluznice po zaužitju nekaterih zdravil. Razvili smo analizo metodo za določevanje vsebnosti CoQ10 v človeški plazmi in plazmi in tkivih raznih živali. Razvito metodo smo uporabili za vrednotenje biorazpoložljivosti vodotopnega CoQ10, kakor tudi za študij vplivov uporabe obogatenih krmil na uspešnost hranjenja kokoši.

Za vodotopno obliko koencima Q10 smo v letu 2006 vložili nacionalne patentne prijave v Evropi, ZDA, Rusiji in Izraelu. Za ta izum smo prejeli zlato priznanje Gospodarske zbornice Slovenije in sklenili licenčno pogodbo za proizvodnjo in trženje vodotopne oblike koencima Q10 v Sloveniji in tujini. V letu 2006

- 1 Patent
- 3 Undergraduate Theses

IMPORTANT ACHIEVEMENTS IN 2006

Research activities in LO6 were oriented toward food and analytical chemistry and, together with partners from industry, also on the evaluation of new pharmaceutical products and active substances where our projects were focused in development, optimization, validation and application of new analytical techniques and methods. Separation, spectroscopic and hyphenated techniques were successfully used for quantitative evaluation of food products and pharmaceutical and biological samples.

Together with the partners from other research institutions selected active substances from plants and animals, important for human health, were evaluated. We developed and validated different analytical methods for the quantitative determination of cholesterol, antioxidants, vitamins and provitamins.

Together with the Veterinary clinic we developed a new HPLC-MS method for quantitative evaluation of sugars in the blood. This method was successfully used for evaluating damages produced by some pharmaceutical products on dogs' intestines.

A national patent application for water soluble Coenzyme Q10 was filed in Europe, the USA, Russia and Israel. This invention received the Golden Recognition Award from the Chamber of Commerce of Slovenia. A licensing agreement for the production and marketing of water soluble Coenzyme Q10 in Slovenia and abroad was also made. In 2006, nine products were launched in eight countries on the basis of this patent. The licensing partners were offered professional support as needed to develop products and to set-up production and marketing.

Some new functional food products with increased amount of CoQ10 were prepared and evaluated. Milk, yogurt, kefir, chocolate, and juices were prepared and evaluated with chemical and organoleptic tests, and the stability of

je bilo na tej osnovi lansiranih devet proizvodov v osmih državah. Licenčnim partnerjem smo nudili strokovno podporo za potrebe razvoja proizvodov, vzpostavitve proizvodnje in trženje. Pripravili in ovrednotili smo nekatere funkcionalne prehrabene izdelke CoQ10, kot so mleko, jogurt, med, šumeče tablete, čokoladni izdelki in sokovi. Izdelke smo kemijsko in organoleptično ovrednotili in jim določili stabilnost.

Da bi pripravili stabilne sadne sokove in njihove embalaže, smo v raznih sokovih in koncentratih določevali vsebnost skupnih polifenolov, skupnih antocianov, vitamina C in antioksidativno učinkovitost. Identificirali in določili smo vsebnost posameznih antocianinov, flavonolov in fenolnih kislin. Preizkušali smo uporabnost embalaže s posebnimi antioksidativnimi lastnostmi in sinergistično delovanje specialne embalaže in antioksidativnih dodatkov. Spremembe smo ugotavljali z merjenjem kemijskih parametrov in senzoričnimi določitvami. Sedaj se dogovarjamo za uporabo dobljenih ugotovitev v industrijskem merilu.

S sodelavci z Biotehniške fakultete (Oddelek za agronomijo) Univerze v Ljubljani smo raziskovali naravno odpornost 21 različnih sort zelja proti določenim škodljivim žuželkam. Razvili smo nove kromatografske metode za določanje triterpenoidov v voskih s površin zeljnih listov. S kombinacijo različnih tehnik (TLC, HPLC-UV, LC-MS) smo dokazali prisotnost treh triterpenoidov (lupeola, α -amirina, β -amirina) v teh voskih.

V okviru sodelovanja z raziskovalci z Nacionalnega inštituta za biologijo (Oddelek za raziskovanje sladkovodnih in kopenskih ekosistemov) smo razvili novo TLC metodo za določanje devetih lipidnih razredov na eni silikagelski HPTLC plošči. Metoda je uporabna za raziskovanje sezonske trofodinamike lipidnih razredov različnih organizmov zooplanktona, kar je osnova za razumevanje prenosa energije v prehranski verigi.

V okviru bilateralnega projekta z Republiko

final products was also established.

In order to prepare stable forms of fruit juices and packing material, special test samples were prepared and the content and changes of concentrations of polyphenols, anthocyanins, antioxidant activity and vitamin C were measured. The influence of new packing materials with antioxidant properties and synergistic effects of these new material and antioxidants additives were tested. All juices with added supplements and stored in new antioxidant material scored better than juices without the addition, at the beginning and after storage. Now we are looking for an agreement with food manufacturers for industrial applications of these obtained results.

Within the cooperation with researchers from the Biotechnical Faculty (Department of Agronomy, Ljubljana, Slovenia), we investigated natural resistance of twenty-one different sorts of cabbage against selected harmful insects. We developed new chromatographic methods for the determination of triterpenoids in cabbage epicuticular waxes. A combination of different techniques (TLC, HPLC-UV, LC-MS) enabled us to determine three triterpenoids (lupeol, α -amyryn and β -amyryn) in the studied waxes.

In the frame of cooperation with the group from the National Institute of Biology (Department of Freshwater and Terrestrial Ecosystems Research, Ljubljana, Slovenia) we developed a new TLC method for the separation of nine main lipid classes (hydrocarbons, wax esters, sterol esters, triacylglycerols, free fatty acids, fatty alcohols, sterols, acetone-mobile polar lipids and phospholipids) on a single silica gel HPTLC plate. The method enabled revealing the seasonal trophodynamic of lipid classes of various zooplankton species, which is a key to understanding the energy transfer through aquatic food webs.

In the frame of the bilateral project with R Macedonia we have developed and validated a chromatographic method for the determination of carotenoid lutein in marigolds (*Tagetes* spp). Marigold can be alternative crop on to-

Makedonijo smo razvili in validirali kromatografsko metodo za določanje luteina v žametnici (*Tagetes patula* L). Žametnica je lahko alternativna kultura na tobačnih poljih, ker ugodno vpliva na zemljišče, saj imajo izločki korenin insekticidno delovanje. Cveti žametnice so najbogatejši znani izvor luteina; v zadnjih letih pa so spoznali, da so cveti žametnice esencialni mikronutrient.

Študirali smo ekstrakcijo karotenoida likopena iz paradižnika in paradižnikovih izdelkov, ker smo želeli optimizirati pripravo testne raztopine, ki bi bila skladna s kromatografskim določanjem. Določili smo tudi vsebnost polifenolov v ekstraktih zaradi vpliva polifenolov na obstojnost likopena. Prehranski dodatki z likopenom so lahko sintetskega izvora, zato smo skušali najti razlike med preparati, ki vsebujejo naravni ali pa sintetski likopen.

It's root excretions have insecticidal properties in soil and the flowers are the richest known source of lutein, which has been recently recognized as essential micronutrient.

We studied the extraction of carotenoid lycopene from tomato and tomato products in order to optimize the preparation of a test solution compatible with further chromatographic quantitation. We determined the content of polyphenols in the extracts because of the influence of polyphenols on stability of lycopene. Dietary supplements with lycopene can contain synthetic lycopene, so we tried to find differences between formulations containing natural or synthetic lycopene.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

Cooperation was going on with several Slovenian companies (Lek d.d., Ljubljana, Slovenia; Krka d.d., Novo mesto, Slovenia; Valens int. d.o.o., Ljubljana, Slovenia; Fructal



SLIKA 1
Prozodi, obogateni z vodotopnim CoQ10, izdelani po patentu Kemijskega inštituta

FIGURE 1
Products enriched with water soluble Coenzyme Q10, produced based on the patent owned by the National Institute of Chemistry

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

Sodelovanje je potekalo s slovenskimi podjetji:

- Lek d.d., Ljubljana;
- Krka d.d., Novo mesto
- Valens Int. d.o.o., Ljubljana;
- Perutnina Ptuj;
- Fructal živilska industrija d.d., Ajdovščina;
- Pivovarna Union d.d., Ljubljana;
- BIA Separations d.o.o., Ljubljana.

In z institucijami:

- Klinični center, Ljubljana;
- Veterinarska fakulteta, Univerza v Ljubljani;
- Veterinarska klinika, Ljubljana;
- Zavod za zdravstveno varstvo Maribor;
- Biotehniška fakulteta, Univerza v Ljubljani;

d.d., Ajdovščina, Slovenia; Pivovarna Union d.d., Ljubljana, Slovenia; BIA Separations d.o.o., Ljubljana, Slovenia) and institutions (Medical Centre Ljubljana, Slovenia; Veterinary Faculty, University of Ljubljana, Slovenia; Veterinary clinic, Ljubljana, Slovenia; Biotechnical Faculty, University of Ljubljana, Slovenia; Institute for Public Health Maribor, Slovenia; National Institute of Biology, Ljubljana, Slovenia).

INTERNATIONAL COLLABORATION

- European project: "New curriculum models for educating food engineers" (TEMPUS-CD_JEP-40065-2005), 2006-2009.
- Bilateral project: Slovenia – Serbia and Montenegro: "Chromatographic Methods in Analysis of Pharmacologically Active Compounds, Investigation of QSPR and QSAR" with the University of Belgrade, Faculty of Pharmacy (Belgrade, Serbia and Monte-



SLIKA 2

Pilotne raziskave postopka za proizvodnjo vodo-topnega koencima Q10 po patentu Kemijskega inštituta

FIGURE 2

Pilot research process for production of water soluble Coenzyme Q10, based on the patent owned by the National Institute of Chemistry

- Inštitut za varovanje zdravja, Ljubljana;
- Nacionalni inštitut za biologijo, Ljubljana itd.

MEDNARODNO SODELOVANJE

- Evropski projekt: "Novi kurikularni modeli za izobraževanje prehrabnenih tehnologov" (TEMPUS-CD_JEP-40065-2005), 2006-2009.
- Bilateralni projekt Slovenija-Srbija in Črna gora z University of Belgrade, Faculty of Pharmacy (Beograd): »Kromatografske metode v analizi farmakološko aktivnih substanc, proučevanje korelacije strukture teh substanc s fizikalno kemijskimi lastnostmi (QSPR) ter z njihovo biološko aktivnostjo (QSAR)«, nosilki: I. Vovk in D. Agbaba.
- Bilateralni projekt Slovenija-Makedonija z University of St. Kliment Ohridski (Bitola), Tobacco Institute (Prilep): »Uvajanje novih rastlinskih kultur z biološko aktivnimi komponentami, zanimivimi za prehrabeno

negro); principal researchers: I. Vovk and D. Agbaba.

- Bilateral project: Slovenia – Macedonia: "Introduction of New Crops with Biologically Active Compounds Interesting for the Food and Pharmaceutical Industry" with the University of St. Kliment Ohridski (Bitola), Tobacco Institute (Prilep); principal researchers: B. Simonovska and K. Filiposki.

MAJOR EQUIPMENT

The laboratory for food chemistry is equipped with HPLC systems with different types of detectors, also with MS detector LCQ from Finnigan; GC systems with different type of injectors (also Head Space injector); complete system for TLC with densitometer, image analyzing system, and automatic applicators; two systems for capillary electrophoresis.



SLIKA 3

HPLC-MS sistemi v Laboratoriju za prehrabeno kemijo

FIGURE 3

HPLC-MS systems, located in Laboratory for Food Chemistry

in farmacevtsko industrijo«, nosilca: B. Simonovska in K. Filiposki.

POMEMBNI INŠTRUMENTI IN OPREMA

Raziskovalci v L06 imajo na razpolago sodobno analizno opremo. Laboratorij je opremljen:

- s HPLC sistemi z različnimi detektorji, med njimi je tudi HPLC-MS sistem Finnigan LCQ;
- z GC sistemi opremljenimi z različnimi tipi injektorjev (med njimi tudi s head-space injektor do 210 °C) in detektorjev;
- s prenosnimi GC sistemi, ki so opremljeni tako, da omogočajo analizo plinov in ogljikovodikov na terenu;
- s kompletno TLC opremo, z avtomatskimi nanašalci, denzitometrom in sistemom za video dokumentacijo.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

V letu 2006 so tri študentke s Fakultete za kemijo in kemijsko tehnologijo, Univerza v Ljubljani, opravile praktični del diplome in tudi diplomirale.

Gostovanja tujih raziskovalcev: dr. Marija Srbinoska, University of St. Kliment Ohridski, Bitola in Tobacco Institute, Prilep, Makedonija.

EDUCATION AND IMPORTANT VISITS

Three students from the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia, finished their practical work in our laboratory and took diplomas.

Research visits:

- Dr. Marija Srbinoska, University of St. Kliment Ohridski, Bitola and Tobacco Institute, Prilep, Macedonia.

L07

Laboratorij za polimerno
kemijo in tehnologijo

Laboratory for Polymer
Chemistry and Technology



VODJA / HEAD

Izr. prof. dr. Majda Žigon

RAZISKOVALCI / RESEARCHERS

Dr. Alojz Anžlovar
Dr. Miroslav Huskić
Mag. Edita Jasiukaityte
Dr. Andrej Kržan
Doc. dr. Matjaž Kunaver
Dr. Ida Mav Golež
Dr. Ema Žagar

**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Blaž Brulc
Maja Gričar
Tina Šmigovec (od / since 1. 11. 2006)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Miran Lavrič
Polona Prosen
Meta Skumavc (od / since 4. 9. 2006)
Mirjana Širca



PODROČJA DEJAVNOSTI

Raziskave so potekale v okviru raziskovalnega programa P2-0145-0104 (Polimeri s posebnimi lastnostmi), enega temeljnega in podoktorskega ter štirih aplikativnih projektov, evropske mreže odličnosti, bilateralnih projektov in projektov za naročnike.

Področja dejavnosti L07 so:

- biorazgradljivi polimeri,
- visoko razvejeni polimeri,
- polimeri iz obnovljivih surovin,
- prevodni polimeri in prevodne kompozitne polimerne membrane iz temperaturno obstojnih polimerov s polarnimi nosilci naboja,
- nanodelci, polimerni nanokompoziti,
- samočistilni fotokatalitski premazi,
- premazni sistemi z nizko vrednostjo HOS,
- recikliranje sintetičnih polimerov,
- lastnosti polimerov in polimernih materialov,
- razvojne raziskave in storitve, predvsem na področju veziv, termoplastov in recikliranja,
- analiza in karakterizacija komercialnih polimerov s spektroskopskimi (FTIR, NMR), kromatografskimi (GC, GC-MS, IGC, SEC, SEC-MALS) in termičnimi (DSC) metodami za naročnike.

RESEARCH ACTIVITIES

Research was conducted in the frame of the research Programme P2-0145-0104 (Specialty Polymers), one basic and four applied projects, two European projects (5.FP), European Network of Excellence (6.FP), five bilateral research projects, and projects with industrial partners. The research activities of L07 are:

- Biodegradable polymers
- Hyperbranched polymers
- Polymers from renewable resources
- Conductive polymers based on substituted polyanilines and composite polymer membranes made of thermally resistant polymers with polar charge carriers
- Nanoparticles, polymer-based nanocomposites
- Self-cleaning photocatalytic coatings
- Coating systems with low VOC content plastics
- Recycling of synthetic polymers
- Properties of polymers and polymeric materials
- Applied and development research, especially for industry of binders, thermoplastics, and recycling

BIBLIOGRAFIJA

- 11 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 2 strokovna članka
- 1 drugo učno gradivo
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanja)
- 8 objavljenih znanstvenih prispevkov na konferencah
- 1 objavljeni strokovni prispevek na konferenci
- 23 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 2 patentni prijavi
- 3 patenti
- 1 prispevek na konferenci brez natisa
- 1 vabljeni predavanja na konferenci brez natisa
- 1 elaborat, predštudija, študija
- 3 diplome
- 5 uredništev revij

GLAVNI DOSEŽKI V LETU 2006

- Biorazgradljivim amfifilnim kopolimerom iz asparaginske kisline in laktida, poli(sukcinimid-ko-laktid)om (PLS) smo določili absolutna povprečja molskih mas in drugi virialni koeficient s statičnimi meritvami sipanja svetlobe (SLS).
- Na področju polimerov iz obnovljivih surovin smo optimizirali postopek utekočinjanja lesa z uporabo koncentrirane žveplove (VI) kisline kot katalizatorja in dosegli več kot 95 % izkoristek, krajši čas in nižjo temperaturo utekočinjanja. Uporabo utekočinjenega lesa kot surovino za sintezo polimerov smo predstavili na prireditvi Hevreka 2006, na Mesecu oblikovanja »Sit in the Sitty« pa smo predstavili prve vzorčne izdelke – stole iz poliuretanske pene.
- V kombinaciji z melaminskimi smolami smo utekočinjeni les uporabili kot vezivo za izdelavo vezanih in ivernih plošč, katerih mehanske lastnosti so enakovredne tistim s komercialnim vezivom, prednost pa je tudi nižja temperatura utrjevanja in s tem

- Analysis and characterization of commercial polymers by spectroscopic (FTIR, NMR), chromatographic (GC, GC-MS, IGC, SEC, SEC-MALS) and thermal techniques (DSC)

BIBLIOGRAPHY

- 11 Original Scientific Articles
- 1 Review Article
- 2 Professional Articles
- 1 Other Educational Material
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 8 Published Scientific Conference Contributions
- 1 Published Professional Conference Contribution
- 23 Published Scientific Conference Contribution Abstracts
- 2 Patent Applications
- 3 Patents
- 1 Unpublished Conference Contribution
- 1 Unpublished Invited Conference Lecture
- 1 Treatise, Preliminary Study, Study
- 3 Undergraduate Theses
- 5 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2006

- Absolute molar masses and the second virial coefficients of biodegradable amphiphilic copolymers made from aspartic acid and lactide, poly(succinimide-colactide)s, PSL, determined by static light scattering measurements.
- Nanofiller montmorillonite (MMT) modified by quaternary polyesters based on an aliphatic acid and alkyldiethanolamine, intended for the preparation of polymeric nanocomposites.
- ZnO and Cu₂O with particle sizes between 100 and 500 nm synthesized by the polyol procedure in di(ethylene glycol), tetra(ethylene glycol) and propylene glycol. Particles of the smallest sizes (100 nm) were obtained at the precursor concentration of 0.1 mol/L. In di(ethylene glycol) 100 – 200 nm

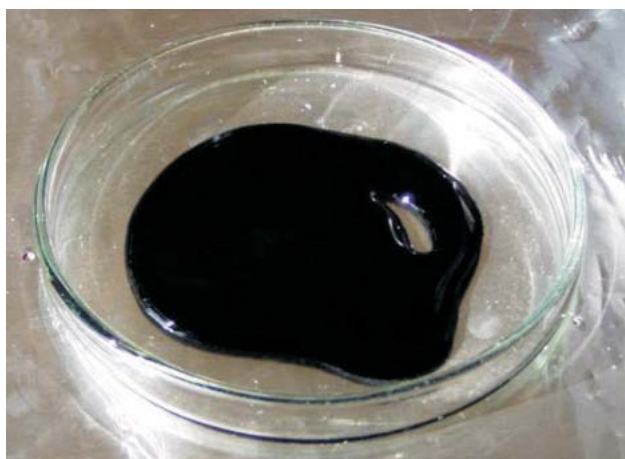
- prihranek na energiji. Potekajo tudi preliminarnе raziskave o uporabi utekočinjenega lesa kot alternativnega goriva.
- Nanopolnilo montmorilonit (MMT) smo modificirali s kvarterniziranimi poliestri na osnovi alifatske kisline in alkildietanolamina. V nadaljevanju bomo modificirane MMT uporabili za pripravo polimernih nanokompozitov.
 - Nanodelce ZnO in Cu₂O velikosti 100–500 nm smo sintetizirali po poliolnem postopku v dietilenglikolu, tetraetilenglikolu in 1,2-propandiolu. Najmanjši delci (100 nm) so nastali pri koncentraciji prekursorja 0,1 mol/L. Nanožičke Cu₂O smo sintetiziral v dietilenglikolu.
 - Z dvema vzorcema laboratorijsko sintetiziranega ZnO (100 nm in 300 nm) in komercialnim vzorcem ZnO (400–600 nm) smo pripravili nanokompozite iz polimetilmetakrilata (PMMA) po postopku polimerizacije v masi. Laboratorijsko sintetizirani delci ZnO so brez modifikacije površine delcev zelo homogeno porazdeljeni po polimerni matrici, medtem ko so delci komercialnega ZnO združeni v skupke. To potrjuje, da imajo ostanki diola na površini delcev funkcijo organofilnih modifikatorjev. Učinki UV absorpcije in termične stabilizacije so zelo odvisni od velikosti delcev: nanokompoziti z ZnO delci velikosti pod 100 nm imajo višjo UV absorpcijo in so termično stabilnejši.
 - Nanokompozite iz polimetilmetakrilata (PMMA) in komercialnih vzorcev modificiranega MMT (Nanofil, Süd Chemie) smo pripravili z interkalacijo v raztopini topil z različno polarnostjo. Z zniževanjem polarnosti topila se je v odvisnosti od uporabljenega modifikatorja MMT povečevala interkalacija polimera med plasti MMT.
 - Iz poliamida 12 (PA12) in molibden-žveplod (MoSI) nanožičk s koncentracijo 0,1 %, 0,3 % in 0,5 % smo pripravili nanokompozite po postopku interkalacije iz taline. Primerjava mehanskih in triboloških lastnosti nanodolgih in 10 – 50 nm debelih Cu₂O nanowires were synthesized.
 - Two samples of ZnO (100 nm and 300 nm) synthesized in our laboratory and a commercial sample (400 – 600 nm) were used in the preparation of PMMA/ZnO nanocomposites by bulk polymerization. ZnO samples synthesized by the polyol procedure are, without any surface modification, homogeneously dispersed through the PMMA matrix while particles of commercial ZnO remain agglomerated. This confirms that polyol residues absorbed at the surface function as organophilic modifiers. Effects of the UV absorption as well as thermal stabilization are strongly dependent on the particle size: nanocomposites with 100 nm ZnO nanoparticles show higher UV absorption and better thermal stabilization compared to samples with 300 nm ZnO.
 - Nanocomposites of poly(methyl methacrylate), PMMA, and commercial modified MMT (Nanofil, Süd Chemie) were prepared by intercalation in solution using solvents of different polarities. It was found that the lower the polarity of the solvent, the better the intercalation, however, it depended also on the type of modifier.
 - Work was continued on the applied project of recycled PET use in the production of resins and coatings. A pilot synthesis (20 kg) of a modified unsaturated polyester resin was done by our industrial partner. The resin gave good test results. We continued with the development of low profile additives on the basis of PET.
 - In cooperation with the Laboratory for molecular modeling and NMR spectroscopy at NIC we developed a new model for the mechanism of microwave heating based on non-equilibrium rotational excitation of reagents. The model was applied in a series of simulations that gave results in agreement with experimental examinations of microwave catalysis.
 - Nanocomposites were prepared in melt from polyamide 12 (PA12) and molybdenum-sul-

kompozitov in PA12 ni pokazala bistvenih razlik.

- Zaradi izjemno močne fotokatalitične aktivnosti titanovega dioksida za razpad umazanije na površinah premazov ostanejo le-ti dalj časa čisti in ohranijo osnovno barvno nianso. V ta namen smo pripravili nanodelce titanovega dioksida s postopkom precipitacije. V pripravi je laboratorijski UV reaktor, s katerim bomo lahko primerjali učinkovitost posameznih formulacij.
- Nadaljevali smo z raziskavami morfologije pigmentiranih premazov, kjer smo z uporabo slikovne analize SEM posnetkov matiranih premaznih površin po selektivnem jedkanju s kisikovo plazmo ugotavljali učinkovitost posameznih matirnih sredstev v praškastih premazih.
- Ugotavljali smo vpliv posameznih pigmentnih mešanic na obstojnost barvne nianse pri premazih, ki jih uporabljamo za izdelavo nacionalnih simbolov. Na osnovi pospešenega staranja premazov in UV obsevanja smo pripravili predloge nekaterih pigmentnih mešanic, ki so primerne za izdelavo nacionalnih simbolov.
- Nadaljevali smo raziskave komercialno dosegljivih visoko razvejenih poliestrov

phur-iodine (MoSI) nanowires concentration of 0.1 %, 0.3 % and 0.5 %. Mechanical and tribological properties of the prepared nanocomposites were comparable to those of pure PA12.

- Due to the extremely strong photocatalytic activity of titanium dioxide causing the degradation of dirt on coating surfaces, these remain clean and retain their original colour. To explore this phenomenon we prepared nanoparticles of titanium dioxide by the precipitation technique. A laboratory UV reactor that will allow the comparison of different formulations is in preparation.
- Studies of the morphology of pigmented coatings were continued. Image analysis of SEM micrographs of matt coating surfaces after selective etching with oxygen plasma allowed the determination of the efficiency of different matting agents in dust coatings.
- We determined the effect of different pigment mixtures on the durability of colour in coatings used in the production of national symbols. Based on accelerated ageing and UV exposure we prepared suggestions of pigment mixtures suitable for national symbols.
- The microstructure and sequence distribution of bacterial poly(3-hydroxybutyrate-co-3-



SLIKA 1:
Utekočinjeni les

FIGURE 1:
Liquified wood

Boltorn treh psevdogeneracij z različnim teoretskim razmerjem jedro/monomer in jih opredelili glede na molsko maso, sestavo in strukturo. Zaradi samokondenzacije monomera kot glavne stranske reakcije pri sintezi Boltorn polimerov nastajajo visoko razvejene strukture brez jedra, ki močno znižajo številčna povprečja molskih mas v primerjavi s teoretičnimi vrednostmi.

- Mikrostrukturo in porazdelitev sekvenc v bakterijskih poli(3-hidroksibutirat-*ko*-3-hidroksivalerat) (PHBV) kopoliestrih smo opredelili s ^{13}C NMR spektrometrijo z analizo diad in triad in z večstopenjsko masno spektrometrijo z elektrorazpršilno ionizacijo (ESI-MSⁿ) ter dobili primerljive rezultate.
- Nadaljevali smo z delom na aplikativnem projektu uporabe recikliranega polietilentereftalata v proizvodnji premazov in plošč. Opravljena je bila pilotna sinteza (20 kg) modificirane nenasičene poliestrske smole pri industrijskem partnerju, ki je uspešno prestala testiranja. Nadaljevali smo z razvijanjem dodatkov smolam, ki preprečujejo skrčke.
- V sodelovanju z Laboratorijem za molekularno modeliranje in NMR spektroskopijo na Kemijskem inštitutu smo razvili nov model mehanizma mikrovalovnega segrevanja, ki temelji na neravnotežnem rotacijskem vzbujanju reaktantov. Model je bil uporabljen v seriji simulacij, katerih rezultati so bili skladni z eksperimentalnimi rezultati mikrovalovne katalize.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Razvojni inštitut, Savatech, Kranj: sodelovanje pri raziskovalnem programu in projektu ter razvojno investicijskem projektu (Evropski sklad za regionalni razvoj – ESRR) na področju elastomernih nanokompozitov.
- Julon d.d., Ljubljana, sodelovanje pri razvojno investicijskem projektu (Evropski sklad za regionalni razvoj – ESRR) »MTX – inovativno vlakno prihodnosti«.

hydroxyvalerate) copolyesters (PHBV) was studied by ^{13}C NMR based on dyad and triad analysis and multistage electrospray ionization mass spectrometry (ESI-MSⁿ). Both techniques gave results that were in good agreement for all investigated samples.

- Commercially available Boltorn hyperbranched (HB) polyesters of different theoretical core/monomer ratio were characterized with respect to molar mass, composition, and structure. Due to monomer self-condensation as the main side reaction in the synthesis of Boltorn polymers HB structures without a core molecule are formed. Since they are of lower molar masses than HB structures with a core molecule, they particularly decrease the number average of molar masses as compared to the theoretically ones.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Research & Technology Institute, Savatech, Kranj, Slovenia: Elastomer-based nanocomposites (research program and project, development & industrial project, European funds for regional development).
- Julon d.d., Ljubljana, Slovenia: MTX – innovative fibre for the future, development & industrial project, European funds for regional development.
- Lek, pharmaceuticals d.d., Ljubljana, Slovenia: research & development project.
- Color d.d., Medvode, Slovenia: The use of waste polymeric materials (applied project).
- KLI Logatec, Slovenia and Biotechnical Faculty, University of Ljubljana, Slovenia: Binders and novel coatings systems with low content of VOC for wood industry (applied project).
- Termo d.d., Škofja Loka, Slovenia: research & industrial project.
- Company in the field of coatings, USA: R&D cooperation.
- Kolpa d.d., Metlika, Slovenia, R&D cooperation

- Lek farmacevtska družba d.d., Ljubljana, raziskovalno razvojno sodelovanje.
- Color d.d., Medvode: sodelovanje pri aplikativnem projektu na področju uporabe odpadnih polimernih materialov.
- KLI Logatec in Biotehniška fakulteta Univerze v Ljubljani: sodelovanje pri aplikativnem projektu na področju sinteze veziv in razvoja novih premaznih sistemov z nizko vrednostjo HOS za lesno industrijo.
- Termo d.d., Škofja Loka: industrijski projekt na področju izolacijskih materialov.
- Podjetje s področja premazov, ZDA: raziskovalno-razvojno sodelovanje.
- Kolpa d.d., Metlika: raziskovalno - razvojno sodelovanje
- Fakulteta za strojništvo, Univerza v Ljubljani in Institut Jožef Stefan, Ljubljana: raziskovalni projekt na področju polimernih nanokompozitov.
- Institut Jožef Stefan, Ljubljana: aplikativni projekt na področju uporabe visoko reaktivne plazme.
- Tehnološka platforma Napredni materiali in tehnologije.
- Za različne partnerje iz industrije (Julon d.d., Ljubljana; Kolektor d.o.o., Idrija; Proizvodnja kemičnih izdelkov TKK Srpénica d.d., Srpénica; Tekstilna tovarna Okroglica d.d., Volčja Draga; Lek d.d., Ljubljana; Saturnus d.d., Ljubljana itd.) analiziramo polimerne in druge materiale ter rešujemo strokovne probleme.
- Faculty of Mechanical Engineering, University of Ljubljana, Slovenia and Jožef Stefan Institute, Ljubljana, Slovenia: Polymer-based Nanocomposites (research project).
- Jožef Stefan Institute, Ljubljana, Slovenia: Highly Reactive Plasma (applied project).
- Technological platform Advanced Materials and Technologies.
- Analysis of polymeric materials and technical problem solutions for our industrial partners (Julon d.d., Ljubljana; Kolektor d.o.o., Idrija; Proizvodnja kemičnih izdelkov TKK Srpénica d.d., Srpénica; Tekstilna tovarna Okroglica d.d., Volčja Draga; Lek d.d., Ljubljana; Saturnus d.d., Ljubljana – all Slovenia etc.)

INTERNATIONAL COLLABORATION

- Participation in the 6 EC framework program Integrated Project 2006-2009: Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics - Nanobiopharmaceutics
 - Network of Excellence, 6.OP EU, 2004-2008: Nanostructured and Functional Polymer-based Materials and Nanocomposites, NANOFUN-POLY.
- Bilateral projects:
- Croatia, 2005–2006 (Faculty of Chemical Engineering and Technology, University of Zagreb): The Preparation of Polymeric Nanocomposite Using Layered Silicates Modified by Polyions.
 - Czech Republic, 2005–2006 (Faculty of Science, Charles University, Prague): Conjugated polymers with main-chain heteroatoms: Synthesis and properties of semiconducting and conducting polymer blends and composites.

MAJOR EQUIPMENT

- Differential scanning calorimeter Pyris 1, Perkin Elmer
- FTIR spectrometer Spectrum One, Perkin Elmer

MEDNARODNO SODELOVANJE

- Sodelovanje pri projektu 6. OP EU, 2006–2009, Nanoscale functionalities for targeted delivery of biopharmaceutics, Nanobiopharmaceutics.
- Mreža odličnosti, 6. OP EU, 2004–2008: Nanostructured and functional polymer-based materials and nanocomposites, Nanofun-poly.
- Bilateralni projekti:

- Hrvaška (2005–2006), Fakultet kemijskog inženjstva i tehnologije, Sveučilište u Zagrebu: Polimerni nanokompozitni materiali na osnovi montmorilonita.
- Češka (2005–2006), Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Praga: Conjugated polymers with main-chain heteroatoms: Synthesis and properties of semiconducting and conducting polymer blends and composites.

POMEMBNI INŠTRUMENTI IN OPREMA

- diferenčni dinamični kalorimeter Pyris 1, Perkin Elmer,
- FTIR spektrometer Spectrum One, Perkin Elmer,
- plinski kromatograf GC 8700, Perkin Elmer,
- souporaba plinskega kromatografa Hewlett Packard Agilent 6890N z masno selektivnim detektorjem 5973N,
- tekočinski kromatograf z UV, RI (Perkin Elmer, Hewlett Packard) in ELS 2100 (Polymer Laboratories) detektorji za meritve SEC in dvodimenzionalne kromatografije,
- tekočinski kromatograf z detektorjem na sipanje svetlobe (Hewlett Packard, Wyatt
- Gas chromatograph GC 8700, Perkin Elmer
- Joint use of a gas chromatograph Hewlett Packard Agilent 6890N with a mass selective detector 5973N
- Liquid chromatograph with UV, RI (Perkin Elmer, Hewlett Packard), and ELS 2100 detectors (Polymer Laboratories) for SEC measurements and for two-dimensional chromatography
- Liquid chromatograph with a multi-angle light scattering photometer Dawn DSP (Hewlett Packard, Wyatt Technology Corporation) for SEC-MALS measurements
- Joint use of a microwave oven Milestone MLS 1200 Mega
- Joint use of the large Institute's equipment (NMR, XRD, LC-MS, SEM)
- Twin screw extruder Teach-Line ZK 25T with water bath and strand pelletizer, Dr. Collin
- Injection moulding machine Babyplast, Rambaldi+Co

EDUCATION AND IMPORTANT VISITS

Mentorship

- Tanja Breskvar: B.S. thesis (VŠŠ): Synthesis of Low Profile Additive for Unsaturated Poly-



SLIKA 2:
Poliuretanska pena iz utekočinjenega lesa

FIGURE 2:
Polyurethane foam made from liquified wood

- Technology Corporation) za meritve SEC-MALS,
- souporaba mikrovalovne pečice Milestone MLS 1200 Mega,
 - souporaba velike inštitutske opreme (NMR, SEM, XRD, LC-MS),
 - dvopolžni laboratorijski ekstruder Teach-Line ZK 25T z vodno kopeljo in granulatorjem, Dr. Collin,
 - stroj za injekcijsko vbrizgavanje Babyplast, Rambaldi+Co.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Mentorstva, komentorstva:

- Tanja Breskvar: diplomsko delo (VSŠ): *Priprava aditiva za nenasičene poliestre iz recikliranega polietilentereftalata*, Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani.
- Peter Trnovšek: diplomsko delo (VSŠ): *Utekočinjen les kot surovina za izdelavo poliuretanskih pen*, Biotehniška fakulteta, Univerza v Ljubljani.
- Irena Truden: diplomsko delo (VSŠ): *Priprava nanokompozitov PMMA/MMT z enostopenjsko in situ polimerizacijo*, Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani.

Obiski:

V okviru bilateralnega sodelovanja so L07 obiskali (tedenski obiski): prof. dr. Jirí Vohlídal, Charles University, Praga, Češka, in mag. Ivan Brnardić, Univerza v Zagrebu, Hrvaška.

Organizirali smo sestanek izvršnega sveta Evropske polimerne federacije.

Uporaba obnovljivih virov za proizvodnjo materialov

Uporaba obnovljivih virov za proizvodnjo materialov obljublja nove trajnostne in do okolja prijazne materiale. Ta tematika je tudi del raziskovalnih aktivnosti Laboratorija za polimerno kemijo in tehnologijo s posebnim poudarkom na uporabi lesa. Les je eden najbolj razširjenih obnovljivih virov in je kljub kompleksni

ters from Recycled Polyethylene Terephthalate, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia.

- Peter Trnovšek: B.S. thesis (VSŠ): *Polyurethane Foams from Liquefied Wood*, Biotechnical Faculty, University of Ljubljana, Slovenia.
- Irena Truden: B.S. thesis (VSŠ): *Synthesis of PMMA/MMT Nanocomposites by One Step in-situ Polymerization*, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia.

Visits

Visitors in the frame of bilateral collaboration: Prof. Dr. Jirí Vohlídal, Charles University, Prague, Czech Republic; Ivan Brnardić, M.S., University of Zagreb, Croatia.

We organized a General Assembly meeting of the European polymer federation.

The use of renewable resources for polymeric materials production

The use of renewable resources for materials production is expected to yield new sustainable and environmentally friendly materials. This topic is also part of the research activities of the Laboratory for Polymer Science and Technology with a particular focus on the use of wood. Wood is one of the most abundant natural materials, and despite its complex composition it is interesting as a potential renewable feedstock for polymer production. One of the possible routes for achieving this is through liquefaction, where wood is reacted with multifunctional alcohols to yield low molecular mass, liquid products that can be used for polymer synthesis.

In our research native hardwoods were liquefied with different glycols and an acidic catalyst. The liquefaction took place at 150 – 180 °C for 0.5 - 3 h during which more than 95% of the wood was liquefied (Figure 1). Analysis of the products revealed the formation of oligomeric degradation products from wood components.

sestavi interesanten kot obnovljiva surovina za proizvodnjo polimerov. Ena od možnih uporab je preko utekočinjanja kjer les reagira z multifunkcionalnimi alkoholi do tekočih produktov nizkih molskih mas, ki jih lahko uporabimo za sintezo polimerov.

V naših raziskavah smo utekočinili domače vrste lesa listavcev z različnimi glikoli in kislinskim katalizatorjem. Utekočinjanje je potekalo 0.5 – 3 ure pri 150 – 180°C, pri čemer se je utekočinilo več kot 95 % začetnega lesa (Slika 1). Analiza produktov je potrdila tvorbo oligomernih degradacijskih produktov iz lesnih komponent. V naslednjem koraku smo utekočinjen les uporabili kot osnovo za sintezo nasičenih in nenasičenih poliestrov. Nenasičene poliestre smo pripravili z reakcijo utekočinjenega lesa z maleinsko in ftalno kislino. Smole razredčene s stirenom so imele zadovoljivo reaktivnost in so vsebovale do 25 % lesa (v suhi snovi). Z uporabo adipinske kisline smo pripravili poliestrske polirole s hidroksilnimi števili med 150 in 500. V reakciji z izocianati so dali serijo poliuretanskih pen, ki imajo lastnosti primerljive s komercialnimi penami in bi bile lahko uporabljene v kmetijstvu in hortikulturi.

In the next phase liquefied wood was used as the basis for synthesis of unsaturated and saturated polyesters. Unsaturated polyesters were prepared by reacting liquid wood with maleic and phthalic acids. Resins diluted by styrene showed satisfactory reactivity and contained up to 25 % wood in dry matter. Using adipic acid we prepared polyester polyols with hydroxyl numbers in the range 150 – 500. These were reacted with isocyanates to give a series of polyurethane foams that were comparable with commercial foams and could be used in agriculture and horticulture (Figure 2).

L08

Laboratorij za organsko sintezo
in kemijo zdravil

Laboratory for Organic and
Medicinal Chemistry



VODJA / HEAD

Dr. Barbara Mohar

RAZISKOVALCI / RESEARCHERS

Dr. Jože Kobe

Dr. Michel Stephan (polovični čas / part time)

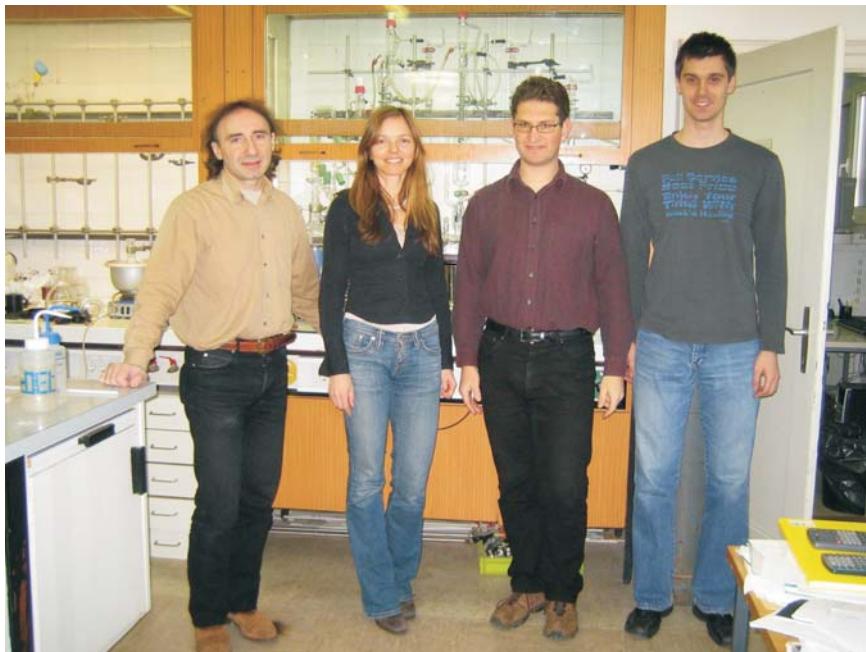
**MLADI RAZISKOVALEC /
YOUNG RESEARCHER**

Damjan Šterk

Borut Zupančič

PRIPRAVNIK / TRAINEE

Jure Kokalj (do / until 31. 7. 2006)



PODROČJA DEJAVNOSTI

- Razvoj novih metodologij v asimetrični sintezi in katalizi,
- sinteza kiralnih spojin s potencialno biološko aktivnostjo,
- razvoj novih sintetskih poti za industrijsko zanimive spojine.

BIBLIOGRAFIJA

- 3 izvorni znanstveni članki
- 3 patentne prijave
- 2 patenta
- 1 uredništvo revije

GLAVNI DOSEŽKI V LETU 2006

- Asimetrično transfer hidrogeniranje fluoroalkil ketonov v visokih enantiomernih presežkih in visokimi izkoristki s kiralnimi amin-sulfamoilamidnimi Ru-katalizatorji razvitimi v našem laboratoriju.
- Razvoj asimetričnega transfer hidrogeniranja p-fluoroacetofenonskih intermediatov za farmacevtsko učinkovino z anti-holesterolnim delovanjem.

RESEARCH ACTIVITIES

- Development of new methodologies in asymmetric synthesis and catalysis.
- Synthesis of chiral compounds with potential biological activity.
- Finding new synthetic routes for industrially interesting compounds.

BIBLIOGRAPHY

- 3 Original Scientific Articles
- 3 Patent Applications
- 2 Patents
- 1 Journal Editorship

IMPORTANT ACHIEVEMENTS IN 2006

- Asymmetric transfer hydrogenation of fluoroalkyl ketones in high enantiomeric excesses with our laboratory developed chiral amine-sulfamoylamide Ru-catalysts.
- Development of asymmetric transfer hydrogenation of p-fluoroacetophenone intermediates for a pharmaceutical ingredient with anti-holesterolemic action.
- Preparation of new chiral phosphane ligands

- Priprava novih kiralnih fosfanskih ligandov in njihovih Rh-kompleksov, ki so pokazali visoko enantioselektivnost in aktivnost pri asimetričnem hidrogeniranju funkcionaliziranih C=C vezi.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Krka, tovarna zdravil d.d., Novo mesto; Razvoj neodvisnih postopkov do farmacevtskih intermediatov.
- Lek farmacevtska družba d.d., Ljubljana; Sinteza potencialnih farmacevtskih učinkovin.
- PhosPhoenix SARL, Pariz, Francija; Razvoj novih industrijskih procesov na osnovi homogene katalize.

MEDNARODNO SODELOVANJE

- Slovensko-francoski bilateralni projekt PROTEUS, 2004–2006 (Univerza Louis Pasteur,

and their Rh-complexes which showed high enantioselectivity and activity in asymmetric hydrogenation of functionalized C=C bonds.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Krka Pharmaceuticals, d.d., Novo mesto, Slovenia: Development of new synthetic routes to selected pharmaceutical intermediates.
- Lek Pharmaceuticals, d.d., Ljubljana, Slovenia: Synthesis of potential pharmaceutical compounds.
- PhosPhoenix SARL, Paris, France: Development of industrial processes based on homogeneous catalysis.

INTERNATIONAL COLLABORATION

- Slovenian-French bilateral project PROTEUS, 2004-2005 (University of Louis Pasteur, Strasbourg, France): New Supported Catalysts for Asymmetric Transfer Hydrogenation.



SLIKA 1:
Destilacija brezvodnih topil

FIGURE 1:
Distillation of dry solvents

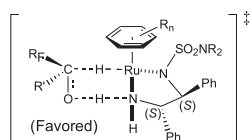
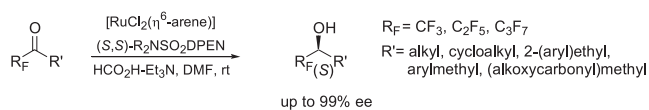
Strasbourg, Francija): Novi katalizatorji za asimetrično transfer hidrogeniranje vezani na naosilec.

POMEMBNI INŠTRUMENTI IN OPREMA

- HPLC in GC sistemi opremljeni s kiralnimi kolonami,
- polarimeter,
- ultra kriomat (-100 do +100 °C),
- sistem za hidrogeniranje (do 100 atm H₂).

MAJOR EQUIPMENT

- HPLC and GC systems equipped with chiral columns
- Polarimeter
- Ultra kryomat (-100 to +100 °C)
- System for hydrogenation (up to 100 atm H₂)



SHEMA 1

Splošen način poteka asimetričnega transfer hidrogeniranja fluoroalkil ketonov kataliziranega z [Ru(*h*⁶-aren)((*S,S*)-R₂NSO₂DPEN)]

SCHEME 1

General sense of asymmetric transfer hydrogenation of fluoroalkyl ketones catalysed by [Ru(*h*⁶-arene)((*S,S*)-R₂NSO₂DPEN)]

L09

Laboratorij za anorgansko kemijo
in tehnologijo

Laboratory for Inorganic Chemistry
and Technology



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dr. Gregor Mali
dr. Alenka Ristić
dr. Maja Mrak (do / until 16.6.2006)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

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Matjaž Mazaj

TEHNIČNO OSEBJE / TECHNICAL STAFF

Olga Gorše
Edi Kranjc
Mojca Opresnik



PODROČJA DEJAVNOSTI

Raziskave poroznih materialov:

- zeolitni materiali,
- mezoporozni materiali,
- cement.

Strukturna analiza materialov:

- rentgenska difrakcija,
- spektroskopija z jedrsko magnetno resonanco
- rentgenska absorpcijska spektroskopija.

<http://www.ki.si/index.php?id=I-09>

BIBLIOGRAFIJA

- 12 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 2 strokovna članka
- 9 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 3 predavanja na tujih univerzah
- 3 uredništva revij

GLAVNI DOSEŽKI V LETU 2006

Raziskave poroznih materialov:

S prehodnimi kovinami modificirane mikroporozne silikate (velikost por od 0.5 do 2

RESEARCH ACTIVITIES

Investigations on porous materials:

- zeolitic materials
- mesoporous materials
- cement research

Materials structural analysis:

- X-ray diffraction
- nuclear magnetic resonance spectroscopy
- X-ray absorption spectroscopy

BIBLIOGRAPHY

- 12 Original Scientific Articles
- 1 Review Article
- 2 Professional Articles
- 9 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 3 Invited Lectures at Foreign Universities
- 3 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2006

Investigations of porous materials:

Transition-metal modified microporous silicates (zeolites) with pore openings from 0.5 to 2 nm are widely used as heterogeneous catalysts in

nm) uporabljamo kot okolju prijazne heterogene katalizatorje pri reakcijah oksidacij. Vgradnja prehodnih kovin v porozno silikatno ogrodje povzroči nastanek katalitsko aktivnih mest. Katalitske lastnosti takšnih materialov so odvisne od njihovega strukturnega tipa ter narave vgrajene kovine in njenega mesta vgradnje v ogrodje. Mezoporozni silikati (premer por od 2 do 10 nm) omogočajo udeležbo v katalitskih reakcijah tudi molekulam večjih dimenzij, vendar je njihova temperaturna stabilnost slabša in ne dosegajo katalitskih lastnosti mikroporoznih silikatov. Naše raziskave so usmerjene v pripravo novih mikroporoznih/mezoporoznih kompozitnih materialov, ki združujejo dobre katalitske lastnosti in temperaturno stabilnost mikroporoznih ter dimenzije por mezoporoznih materialov. Sintetizirali smo mikroporozne/mezoporozne kompozitne silikate modificirane s titanom. Mikroporozno in mezoporozno strukturo smo raziskali z rentgensko difrakcijo in transmisijskim elektronskim mikroskopom z visoko ločljivostjo. Lokalno okolico titana v silikatnem ogrodju smo določili z rentgensko absorpcijsko spektroskopijo. Rezultati karakterizacije kažejo na termično obstojne mikroporozne/mezoporozne kompozitne materiale s katalitsko aktivnimi mesti titana.

Naravne zeolite uporabljajo pri odstranjevanju amoniaka in težkih kovin iz odpadnih in pitnih voda. V sodelovanju z Univerzo v Zagrebu smo preučili možnosti odstanjevanja cinka iz odpadnih vod galvanske industrije z metodo rentgenske difrakcije na praškastih vzorcih ter komplementarnih analitskih metod, predvsem jedrske magnetne resonance in rentgenske absorpcijske spektroskopije.

Za Salonit Anhovo, d.d., Deskle smo zaključili raziskave vplivov 10 in 20 % dodatka kalcita na hidratacijo Portlandskega cementa. Časi hidratacije so bili 1, 3, 7, 15, 28 in 90 dni pri temperaturah 25 in 40 °C. Raziskali smo tudi vpliv 20 % dodatka kalcita različnih granulacij ($d_{sr} = 20,5, 12,0, 1,6$ in $0,83$ mm) na potek hidratacije v 15, 28 in 90 dneh pri 25 °C.

oxidation reactions. These catalysts exhibit remarkable catalytic activity due to transition-metal centers that are isolated in the silicate framework. Catalytic properties of these materials depend on the structure type, location and the nature of incorporated metal. The pore size limitations of microporous catalysts can be overcome by using mesoporous silicates with pore openings from 2 to 10 nm when larger reactants have to be processed. However, mesoporous species do not exhibit excellent catalytic properties of microporous silicates.

Our research was focused on the preparation of novel microporous/mesoporous composite silicates that combine good catalytic properties and thermal stability of microporous and pore openings of mesoporous silicates. We have synthesized microporous/mesoporous silicates modified by the titanium. Microporous and mesoporous structures were investigated by X-ray powder diffraction and High Resolution Transmission Electron Microscopy. Local environment of the titanium in the silicate framework was identified by X-ray absorption spectroscopy. The results of characterization indicated thermal stability of prepared microporous/mesoporous composite silicates with catalytically active titanium centres.

Natural zeolites have been used for the removal of ammonia and heavy metals from drinking water and wastewaters. With the University of Zagreb, Croatia we explored the possibilities for the zinc removal from wastewaters of galvanic industry using X-ray powder diffraction methods and complementary methods with the emphasis on nuclear magnetic resonance and X-ray absorption spectroscopy.

The research performed for Salonit Anhovo d.d., Deskle, Slovenia on the effects of 10 and 20 % addition of calcite on the hydration of Portland cement was completed. The investigation was carried out during different times of hydration (1, 3, 7, 15, 28 and 90 days) at two temperatures (25 and 40 °C). The study of the influence of a 20 % addition of calcite, having different particle size distributions ($d_{med.} = 20,5,$

Hidratizirane faze in njihove vsebnosti smo ovrednotili z rentgensko praškovno difrakcijo, termogravimetrično analizo ter infrardečo spektroskopijo. Dodatki kalcita vplivajo na nastanek in vsebnost specifičnih faz, čas hidratacije pa na fazno sestavo ter mikrostrukturo hidratiziranega cementa.

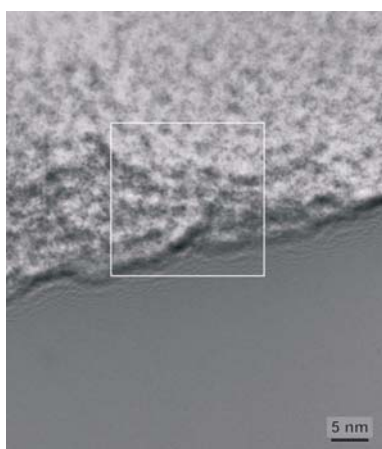
Iz TG (ASTM E1641) in DSC krivulj (metoda Flynn-Wall-Ozawa) smo določili karakteristike kinetičnega razpada (E_a , kJ/mol in A , min⁻¹) tetrakalcijevega monokarboaluminata 11-hidrata, ki nastaja v hidratiziranih cementih z dodatkom apnenca.

Strukturna analiza materialov:

Z metodo rentgenske praškovne difrakcije in rentgenske difrakcije na monokristalih smo določili strukture novih poroznih organokovinskih spojin na fosfatni osnovi, kot

12.0, 1.6 and 0.83 mm), on the phase composition of hydrated Portland cement after 15, 28 and 90 days was also performed. Hydrated phases and their contents were evaluated and quantified by powder X-ray diffraction, thermogravimetric analysis and infrared spectroscopy. The additions of calcite influenced the formation and contents of specific phases, whereas hydration times mainly affected final phase compositions and the overall microstructure of hydrated cement.

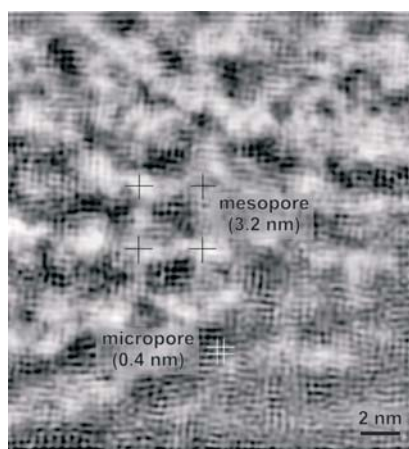
The kinetic constants (E_a , kJ/mol and A , min⁻¹) for the thermal decomposition of tetracalcium monocarboaluminate 11-hydrate that forms during the hydration of calcite-containing cement were determined from thermogravimetric and DSC curves by ASTM E1641 and Flynn-Wall-Ozawa method, respectively.



a)

SLIKA 1:

a) Fotografija presečne elektronske mikroskopije visoke ločljivosti (HRTEM) mikroporoznega/mezoporoznega (Ti,Al)-Beta/MCM-48 silikatnega kompozita s popačeno kubično razporeditvijo mezopor. b) Izsek slike a) filtriran s pomočjo Fourierjeve transformacije prikazuje delokalizirano ureditev mikropor v mezoporozni matrici.



b)

FIGURE 1:

(a) High Resolution Transmission Electron Microscopy (HRTEM) image of microporous/mesoporous (Ti,Al)-Beta/MCM-48 silicate composite with a distorted cubic arrangement of mesopores. The corresponding electron diffraction pattern (inset) reveals the presence of microporous domains. (b) FFT filtered image of the inset from Figure 1(a) shows a delocalised micropore pattern having narrower lattice spacing than the hosting mesoporous matrix.

potencialnih adsorbentov za uporabo pri skladiščenju vodika.

Z jedrsko magnetno resonanco smo pomagali karakterizirati mezoporozne aluminofosftane materiale in mikro-mezoporozne silikatne kompozitne materiale. Razvili smo metodo za študij korelacij med dipolno sklopljenimi kvadrupolnimi jedri, npr. med jedri aluminija v aluminofosfatih, ki uporablja močna radiofrekvenčna polja. Mehanizem delovanja metode ni povzet po metodah za preprostejše sisteme sklopljenih jeter s spinom 1/2, temveč je specifičen za kvadrupolna jedra.

Z magnetno resonanco smo študirali tudi zgradbo zanimivih litijevih spojin, ki bodo v bodoče lahko izboljšale lastnosti litijevih baterij, in sistematično raziskovali spreminjanje kemijskega premika vodikovega jedra in kemijskega premika v kvadrupolne sklopitvene konstante devterijevega jedra v prisotnosti različno močnih vodikovih vezi.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Salonit Anhovo, d.d., Deskle: raziskave in razvoj cementov z apnencem in mineralnimi dodatki
- Krka d.d., Novo mesto: rentgenska praškovna analiza in določanje specifične površine

MEDNARODNO SODELOVANJE

- Šesti okvirni program Evropske unije, NoE FP6 INSIDE PORES (2004-2008), Coordinator: National Center for Scientific Research "Demokritos", Atene, Grčija
- ESRR – Evropski sklad za regionalni razvoj, Center odličnosti "Nanoznanosti in nanotehnologije" (2004–2006)
- ESRR – Evropski sklad za regionalni razvoj, NMR center odličnosti za študij struktur in interakcij v biotehnologiji in farmaciji (2004–2006)
- Slovensko-francoski bilateralni projekt, PROTEUS (2005–2006), Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, Francija

Materials structure analysis:

X-ray powder and single-crystal diffraction were used for the crystal structure determination of new porous phosphate-based inorganic-organic compounds as potential adsorbents for their use in hydrogen storage.

Nuclear magnetic resonance was used for the characterization of mesoporous aluminophosphate and micro-mesoporous silicate composite materials. We developed a method for studying correlations between dipolar-coupled quadrupolar nuclei, e.g. between aluminium nuclei within aluminophosphates. The method employs strong radiofrequency fields. It is designed specifically for half-integer quadrupolar nuclei and it is not adopted from techniques for simpler systems of coupled spin-1/2 nuclei. Magnetic resonance was also used for studying structural properties of interesting lithium compounds that could substantially improve characteristics of lithium batteries in the future. We have also systematically studied changes in the isotropic chemical shift of hydrogen and deuterium nuclei and changes in quadrupolar coupling constant of deuterium nuclei participating in hydrogen bonds of various strengths.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Salonit, Anhovo d.d., Deskle, Slovenia: investigations and development of cements with limestone and mineral admixtures
- Krka d.d., Novo mesto, Slovenia: X-ray powder diffraction analyses and the determination of specific surface areas

INTERNATIONAL COLLABORATION

- The 6. Framework Programme of European Union, NoE FP6 INSIDE PORES (2004-2008), Coordinator: National Center for Scientific Research "Demokritos", Athens, Greece
- ERDF – The European Regional Development Fund, Centre of excellence "Nanoscience and nanotechnology" (2004-2006)
- ERDF – The European Regional Development

- Slovensko francoski bilateralni projekt, PROTEUS (2005–2006), Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija
- Slovensko argentinski bilateralni projekt (2006–2008), Unidad de Actividad Quimica, Buenos Aires, Argentina
- Slovensko hrvaški bilateralni projekt (2005–2006), Institut Ruđer Bošković, Zagreb, Hrvaška
- Slovensko srbski bilateralni projekt (2006–2007), Tehnološko-metalurška fakulteta, Beograd, Srbija in Črna Gora
- Projekt z Univerzo v Manchestru v okviru sporazuma o znanstvenem sodelovanju med SAZU in The Royal Society, London, Velika Britanija
- Fund, NMR Centre of excellence for the study of structures and interactions in biotechnology and pharmacy (2004-2006)
- Slovenia-France bilateral project, PROTEUS (2005-2006), Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, France
- Slovenia-France bilateral project, PROTEUS (2005-2006), Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, France
- Slovenia-Argentina bilateral projekt (2006-2008), Unidad de Actividad Quimica, Buenos Aires, Argentina
- Slovenia-Serbia bilateral project (2006-2007), Faculty of Technology and Metallurgy, University of Belgrade, Serbia and Montenegro
- Slovenia-Croatia bilateral project (2005-2006), Ruđer Bošković Institute, Zagreb, Croatia

POMEMBNI INSTRUMENTI IN OPREMA

- Rentgenski praškovni difraktometer Siemens D 5000 (sevanje CuK α z $\lambda = 1.5406\text{\AA}$) za snemanje praškovnih posnetkov visoke ločljivosti, pri visokih temperaturah od 50 do 1450°C, pri nizkih temperaturah od vrelišča dušika do 400°C, v vakuumu ali drugih atmosferah ter snemanje tankih filmov.
- Rentgenski praškovni difraktometer PANalytical X'Pert PRO (sevanje CuK α z $\lambda = 1.5406\text{\AA}$) za snemanje praškovnih posnetkov v štirih različnih konfiguracijah: (1) α_1 z Johannsonovim monokromatorjem za vzorce z ravno površino, (2) kapilarna transmisija z hibridnim monokromatorjem, (3) standardna Bragg-Brentano, (4) paralelni žarek.
- Tristar 3000, avtomatski plinski analizator (Micromeritics Instrument Co.) za merjenje specifične površine (BET), adsorpcijskih izoterm, volumna in porazdelitve por praškastih vzorcev.
- SDT 2960 sistem za termično analizo, DSC-TGA (TA Instruments Inc.) omogoča simultane meritve energijskega pretoka in masnih sprememb v materialih od sobne temperature do 1500°C.

MAJOR EQUIPMENT

- X-ray powder diffractometer Siemens D 5000 (radiation wavelength CuK $\alpha = 1.5406\text{\AA}$) for measurements of powder patterns with high resolution at high temperatures from 50 to 1450 °C, at low temperatures from boiling point of liquid nitrogen to 400 °C in vacuum or other atmospheres and for measurements of thin films.
- X-ray powder diffractometer PANalytical X'Pert PRO (radiation wavelength CuK $\alpha = 1.5406\text{\AA}$) for measurements of powder patterns on four different configuration: (1) α_1 with Johansson monochromator, for flat samples, (2) capillary transmission with Hybrid monochromator, (3) standard Bragg-Brentano, and (4) parallel beam.
- Tristar 3000, an automated gas adsorption

- Sistem za termično nalizo (model TA 2000, TA Instruments Inc.), ki je sestavljen iz TGA (1200°C) in DSC (725°C) modulov.
- Microtrac S3500, aparatura za določevanje velikosti in porazdelitev delcev v mokrem ali suhem stanju. Območje meritev za mokre vzorce od 0,02 μm do 1400 μm in za suhe vzorce od 0,25 μm do 1400 μm .
- AutoPycnometer (Micromeritics Instrument Co.) aparatura za avtomatsko določevanje gostote materialov s helijem.
- Centrifuga Hettich, Rotanta 460 R hlajena (temperaturno območje od -20°C do $+40^{\circ}\text{C}$ analyser (Micromeritics Instrument Co.) for specific surface area (BET) measurements, adsorption isotherms, volume pore and pore size distribution of powder samples (mesopores and macropores: $> 2 \text{ nm}$).
- SDT 2960 system for thermal analysis, DSC-TGA (TA Instruments Inc.) for simultaneous measurements of enthalpy and mass changes in materials (from 30 to 1500°C).
- Microtrac S3500 Particle Size Analyzer, wet or dry samples. The range of measurement for wet samples is from 0.02 μm to 1400 μm (2800 μm) and for dry samples from 0.25



SLIKA 2:

Matjaž Mazaj med meritvami na sinhrotronu ELETTRA (SAXS beamline) z gostujočim raziskovalcem v našem laboratoriju G.J.A.A. Soler-Illia (z leve proti desni: Luca Malfatti – Università di Sassari, Alghero, Italija, G.J.A.A. Soler-Illia – Unidad de Actividad Quimica, Buenos Aires, Argentina, Stefano Costacurta – Università di Sassari, Alghero, Italija, Paolo Falcaro – Università degli Studi di Padova, Padova, Italija, Matjaž Mazaj – Kemijski inštitut, Ljubljana, prof. Plinio Innocenzi, Università di Sassari, Alghero, Italija).

FIGURE 2:

Matjaž Mazaj during measurements at the synchrotron ELETTRA (SAXS beamline) with visiting researcher in our laboratory G.J.A.A. Soler-Illia (from the left: Luca Malfatti – Università di Sassari, Alghero, Italy, G.J.A.A. Soler-Illia – Unidad de Actividad Quimica, Buenos Aires, Argentina, Stefano Costacurta – Università di Sassari, Alghero, Italy, Paolo Falcaro – Università degli Studi di Padova, Padova, Italy, Matjaž Mazaj – National Institute of Chemistry, Ljubljana, Slovenia, Prof. Plinio Innocenzi, Università di Sassari, Alghero, Italy).

- C). Hitrost vrtenja od 500 do 9500 obr/min.
- Ultra Turrax disperzer T25 (IKA).
- Mikrovalovna peč MLS-1200 MEGA (Milestone).
- Mikrovalovna peč ETHOS (Milestone).
- Mlin za mešanje in homogeniziranje prahov, suspenzij in past Retsch RM 100.
- Kalcinacijske peči: dve cevni (segrevanje do 1000°C, hitrost segrevanja 1,5-2°C/min) in ena komorna (segrevanje do 1200°C, hitrost segrevanja 3°C/min).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Izobraževanje:

- dr. Nataša Novak Tušar je bila izvoljena v naziv docent za področje kemije na Univerzi Nova Gorica.

Obiski tujih raziskovalcev:

- dr. G.J.A.A. Soler-Illia, Unidad de Actividad Quimica, Buenos Aires, Argentina
- dr. Michael Stöcker, SINTEF, Norveška
- prof. Mladen Eić, University of New Brunswick, Department of Chemical Engineering, Fredericton, NB Canada
- dr. Frederic Thibault-Starzyk, Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija
- prof. Nevenka Rajić, Tehnološko-metalurška fakulteta, Univerza v Beogradu, Srbija in Črna Gora
- dr. Cleo Kosanović, Institut Ruđer Bošković, Zagreb, Hrvaška
- dr. Sanja Bosnar, Institut Ruđer Bošković, Zagreb, Hrvaška

Gostovanja:

- dr. Maja Mrak je gostovala na Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Nemčija (1 teden)
- Matjaž Mazaj je gostoval na University of Antwerp, Belgija (6 tednov)
- Saša Cecowski je gostovala na Unidad de Actividad Quimica, Buenos Aires, Argentina (3 tedne)

μm to 1400 μm.

- AutoPycnometer (Micromeritics Instrument Co.) for automatic determination of true density of materials with helium.
- High-speed centrifuge, Hettich, Rotanta 460 R, refrigerated (temperature control -20°C to +40°C). Speed control within a range of 500 - 9.500 rpm.
- Ultra Turrax disperser T25 (IKA).
- Microwave oven MLS-1200 MEGA (Milestone).
- Microwave oven ETHOS (Milestone).
- Grinder for mixing and homogenizing powders, suspensions and pastes, Retsch RM 100.
- Furnaces: two tubes (heating up to 1000°C, heating rate 1.5-2 °C/min) and one chamber (heating up to 1200°C, heating rate 3°C/min).

EDUCATION AND IMPORTANT VISITS

Education:

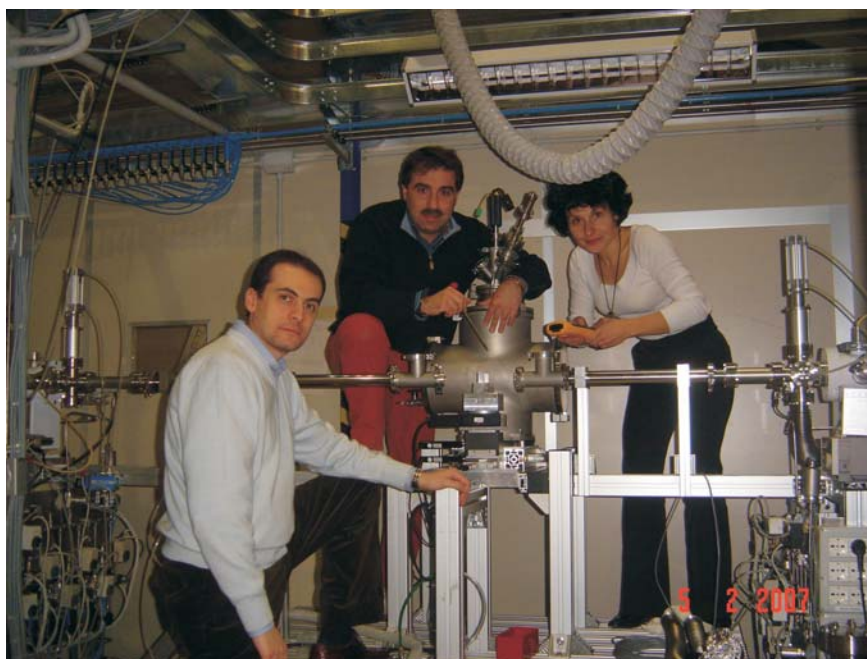
- Dr. Nataša Novak Tušar was elected assistant professor for the field of chemistry at University Nova Gorica, Slovenia

Visits of foreign researchers:

- Dr. G.J.A.A. Soler-Illia, Unidad de Actividad Quimica, Buenos Aires, Argentina
- Dr. Michael Stöcker, SINTEF, Norway
- Prof. Mladen Eić, University of New Brunswick, Department of Chemical Engineering, Fredericton, NB Canada
- Dr. Frederic Thibault-Starzyk, Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, France
- Prof. Nevenka Rajić, Faculty of Technology and Metallurgy, University of Belgrade, Serbia and Montenegro
- Dr. Cleo Kosanović, Ruđer Bošković Institute, Zagreb, Croatia
- Dr. Sanja Bosnar, Ruđer Bošković Institute, Zagreb, Croatia

Visits of foreign institutes:

- dr. Alenka Ristić in dr. Gregor Mali sta gostovala v Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija (2x1 teden)
 - dr. Gregor Mali je gostoval na Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, Francija (1 teden)
 - dr. Nataša Novak Tušar in dr. Alenka Ristić sta gostovali na Institutu Ruđer Bošković, Zagreb, Hrvaška
 - Dr. Maja Mrak visited Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany (1 week)
 - Matjaž Mazaj visited University of Antwerp, Belgium (6 weeks)
 - Saša Cecowski visited Unidad de Actividad Quimica, Buenos Aires, Argentina (3 weeks)
 - Dr. Alenka Ristić and Dr. Gregor Mali visited Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, France (2x1 week)
 - Dr. Gregor Mali visited Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, France (1 week)
 - Dr. Nataša Novak Tušar and Dr. Alenka Ristić visited Ruđer Bošković Institute, Zagreb, Croatia
- V letu 2006 smo pri karakterizaciji materialov uporabljali sinhrotronska sevanja v večjem obsegu kot v prejšnjih letih:
- 1) Sinhrotron ELETTRA (Bazovica, Italija): rentgenska absorpcijska spektroskopija (XAFS beamline) in rentgenska difrakcija pri nizkih kotih (SAXS beamline).



SLIKA 3:

Nataša Novak Tušar med meritvami na sinhrotronu ELETTRA (XAFS beamline) z raziskovalcem na žarkovni liniji Luca Olivi (drugi z leve) in postdoktorskim raziskovalcem Andrea Cognigni (prvi z leve).

FIGURE 3:

Nataša Novak Tušar during measurements at the synchrotron ELETTRA (XAFS beamline) with beamline scientist Luca Olivi (second from the left) and post-doctoral researcher Andrea Cognigni (first from the left).

2) Sinhrotron DESY (Hamburg, Nemčija):
rentgenska absorpcijska spektroskopija (E4
beamline).

3) Institute Laue Langevin (Grenoble, Francija):
neutronska difrakcija (VIVALDI beamline).

Synchrotron radiation tools were used for ma-
terials characterization to a larger extent in
2006 as in previous years:

1) Synchrotron ELETTRA (Basovizza, Italy): X-ray
Absorption Spectroscopy (XAFS beamline) in
Small Angle X-Ray Scattering (SAXS
beamline).

2) Synchrotron DESY (Hamburg, Germany): X-
ray absorption Spectroscopy (E4 beamline).

3) Institute Laue Langevin (Grenoble, France):
Neutron Diffraction (VIVALDI beamline).

L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry



VODJA / HEAD

Doc. dr. Janko Jamnik

RAZISKOVALCI / RESEARCHERS

Dr. Marjan Bele

Dr. Robert Dominko

Doc. dr. Miran Gaberšček

**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Boštjan Erjavec (od / since 1. 11. 2006)

Boštjan Genorio

Mirjana Küzma

Jože Moškon (od / since 1. 11. 2006)

Dušan Strmčnik

TEHNIČNO OSEBJE / TECHNICAL STAFF

Milena Zorko

Gregor Kapun

Marjeta Kebrič (delno / partly)

PRIPRAVNIKI / TRAINEES

Petra Mihelčič



PODROČJA DEJAVNOSTI

Materiali za energijske in informacijske tehnologije, podrobnejša opredelitev:

- študij kinetike transporta in sprememb kemijske sestave v trdnih mešanih prevodnikih;
- vpliv nanostrukturiranosti trdnih kompozitov na izbrane lastnosti, kot so elektrokemijsko shranjevanje energije, raztapljanje, elektrokataliza ipd. (uporaba v energetiki, informatiki, farmaciji);
- priprava in karakterizacija nanometrskih ovojníc okoli funkcionalnih delcev;
- priprava nanometrskih filmov na zunanjih in/ali notranjih površinah funkcionalnih materialov;
- vgradnja funkcionalnih materialov v ustrezne matrike;
- vpliv površinskega naboja na stabilnost disperzij ter suspenzij; polielektrolitske titracije.

BIBLIOGRAFIJA

- 17 izvirnih znanstvenih člankov
- 3 objavljeni znanstveni prispevki na konferencah (vabljen predavanje)

RESEARCH ACTIVITIES

- Materials for energy and information technologies

Detailed classification:

- Study of transport kinetics and chemical composition changes in solid mixed conductors
- Influence of nanostructuring of solid composites on selected properties, such as electrochemical energy storage, dissolution, electrocatalysis etc. (application in energetics, informatics and pharmacy)
- Preparation and characterization of nanometre-sized coatings on functional particles
- Preparation of nanometre-sized film on external or internal surfaces of functional materials
- Incorporation of functional materials into matrices
- Influence of surface charge on stability of dispersions and suspensions; polyelectrolyte titrations

- 21 objavljenih povzетkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 2 prispevka na konferencah brez natisa
- 1 končno poročilo o rezultatih raziskav
- 1 diploma

GLAVNI DOSEŽKI V LETU 2006

Koncept mešanega potenciala za insercijske materiale

Mešani potencial je zelo znan kinetični koncept na področju korozije. Je posledica dveh ali več elektrokemijskih reakcij, ki sočasno potekajo na površini prevodnega, največkrat kovinskega materiala. Neto tok, ki ustreza korozijskemu potencialu, je merilo za hitrost korozije, zato mešani potencial pogosto imenujejo tudi korozijski potencial. V laboratoriju smo ugotovili, da lahko mešani potencial definiramo tudi na področju insercijskih materialov, torej takrat, ko je elektrokemijski potencial definiran z vgradnjo izbrane snovi (litija ipd.) v različne gostujoče materiale, ki so v medsebojnem električnem kontaktu. Pokazali smo, da v tem primeru, zaradi omejene in znane množine reaktantov, mešani potencial lahko celo izpeljemo iz osnovnih termodinamskih zakonov. Izpeljano enačbo lahko koristno uporabimo za eksakten izračun termodinamske napetostne krivulje za poljubno kompozitno insercijsko elektrodo, ki se uporablja bodisi v baterijah bodisi sorodnih napravah.

Kompoziti zdravilnih učinkovin in izbranih anorganskih snovi

Nadzorovano sproščanje zdravilnih učinkovin je eden največjih raziskovalnih izzivov tako na področju farmacije kot materialov. Hitrost raztapljanja učinkovine namreč odločilno vpliva na absorpcijo in prehajanje učinkovin v telo. Ugotovili smo, da se pri pripravi učinkovin z obarjanjem (metoda z zamenjavo topila) zelo spremeni morfologija delcev. Na primer pri obarjanju naproksena se je specifična površina v primerjavi z originalnim (mikroniziranim) vzorcem povečala za okoli faktor 3, za podoben

BIBLIOGRAPHY

- 17 Original Scientific Articles
- 3 Published Scientific Conference Contributions (Invited Lectures)
- 21 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 2 Unpublished Conference Contributions
- 1 Final Research Report
- 1 Undergraduate Thesis

IMPORTANT ACHIEVEMENTS IN 2006

Derivation of mixed potential for insertion materials

Mixed potential is a well-known kinetic concept that is extensively used in corrosion studies. It is a consequence of two or more electrochemical reactions proceeding simultaneously on a conducting (usually metallic) surface. As the corresponding net current is often used as a measure for corrosion rate, the mixed potential is also known as the corrosion potential. We have found that a similar mixed-potential concept can be used for prediction of electrochemical properties of composite insertion materials. There the electrochemical potential is determined by simultaneous insertion of a species (e.g., lithium) into different host materials held in electrical contact. As in insertion materials, unlike in corrosion, the total quantity of reacting species is precisely known, it is even possible to derive the mixed potential from basic thermodynamic laws. The derived equation can be used for accurate prediction of thermodynamic charge-discharge curves for any practical composite battery electrode of interest.

Drug – inorganic material composites for use in pharmacy

Controlled drug release is a major research challenge both in the field of pharmacy as well as in materials science. The rate of drug release has a crucial impact on the drug absorption and its further distribution in body. We have found that a properly controlled precipitation

faktor pa se je povečala tudi hitrost raztapljanja (v kislem mediju).

Poseben izziv predstavlja priprava nanokompozitnih materialov učinkovina-anorganski nosilec. Razvili smo dva tipa takih nanostrukturiranih kompozitov, v obeh primerih smo uporabili sol-gel postopek. V prvem primeru smo "in situ" obložili delce modelne učinkovine s plastjo SiO_2 , v drugem primeru pa smo učinkovino vključili v anorgansko gelsko strukturo. Kot modelni primer za podroben študij kinetike raztapljanja smo uporabili sistem klaritromicin-silicijev dioksid. Tako v primeru SiO_2 oblog na klaritromocinu kot v primeru vgradnje klaritromicina v SiO_2 matriko smo dosegli zadržano sproščanje. Pokazali smo, da so slednji kompoziti še posebej homogeni, če sintezo izvajamo v kapljičnem reaktorju; na ta način lahko precej natančneje reguliramo tako čas kot prostor, v katerem reakcija poteka.

V tretjem segmentu raziskav smo se osredotočili na pripravo materialov, ki bi učinkovito odpravili nezaželene stranske pojave pri uporabi

method essentially modifies the morphology of precipitated drug particles. In particular, the specific surface area of naproxen can be increased by a factor of 3, if compared to the drug prepared according to a conventional procedure. The rate of drug release is increased by a similar factor.

A special challenge is preparation of nanocomposites composed of a drug substances and an inorganic compound. We prepared two types of such composites, in both cases we used modified sol-gel procedures. The first composite consisted of drug particles, each of which was covered uniformly with a micrometre-thick silica layer. In the second case, we incorporated selected drug into a silica gel-like matrix. As the model system for detailed study of release profiles we used well-defined silica-clarithromycine composites. Both the coated-drug and the incorporated-drug types of composites showed significantly decreased release rates with respect to the untreated drug. We have found that the distribution of drug in the inor-



SLIKA 1:
Morfologija naproksena, prekristaliziranega po običajnem postopku. Tipične dimenzije delcev: 20–100 mikrometrov.

FIGURE 1:
Morphology of naproxen prepared according to a standard procedure. Typical particle dimensions: 20 – 100 micrometres.

kovinskih medicinskih vsadkov (implantatov). Na eni strani je potrebno zaščititi vsadke pred korozijo, na drugi pa preprečiti, da telo zazna vsadek kot tujek. Znano je, da bi obe funkciji lahko imeli obloge na osnovi hidroksiapatitov – spojin, ki so sicer glavna sestavina kosti. Izkaže se, da je priprava hidroksiapatitov s kontrolirano sestavo in hkrati kontrolirano morfologijo zelo zahtevna naloga. Kljub temu smo v sodelovanju z Institutom Jožef Stefan uspeli pripraviti goste in tanke hidroksiapatitne obloge, ki za nekaj redov velikosti zmanjšajo hitrost korozije tipičnih kovinskih vsadkov. Pri tem je ključnega pomena, da smo v obloge uspeli vgraditi tudi določeno količino zdravilne učinkovine, ki naj bi ob počasnem sproščanju imela analgetski učinek v postoperativnem obdobju.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Iskra TELA d.d., PE Baterije Zmaj, Šentvid pri Stični: optimizacija baterijskih elektrod;
- Belinka d.d., Ljubljana: študij stabilnosti barvnih suspenzij;
- Lek d.d., Ljubljana: priprava kompozitov s kontroliranim sproščanjem učinkovin;
- Predilnica Litija, partner v Centru odličnosti Nanoznanosti in nanotehnologije, Evropski sklad za regionalni razvoj – ESRR, ukrep 1.1. in 1.4;
- Atotech Podnart, d.d., partner v Centru odličnosti Nanoznanosti in nanotehnologije, ESRR, ukrep 1.1. in 1.4;
- JUB, kemična industrija d.d., Dol pri Ljubljani.

MEDNARODNO SODELOVANJE

- ALISTORE, mreža odličnosti v 6. okvirnem programu Evropske unije;
- Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics (FP6-2004-NMP-NI-4) - NANO(BIOPHARMACEUTICS, Integrirani projekt (Ips) znotraj 6. evropskega okvirnega programa.

ganic matrix is especially homogeneous if the synthesis is carried out in a »droplet-reactor«. This way, the space and time within which the reaction takes place is much easier to control. One research segment was devoted to preparation of protective coatings on metallic medical implants. The coatings are supposed to possess two functions: they should protect the implant against corrosion but must also be biocompatible to prevent reaction of the body against the implant. A good candidate for such coating seems to be hydroxyapatite – a compound that is the main constituent of bones. The problem is that it is very difficult to synthesize hydroxyapatite with a controlled composition and, especially, controlled morphology. In cooperation with Jozef Stefan Institute we have succeeded to prepare thin and dense hydroxyapatite coatings that decrease the corrosion rate of metallic implants by about three orders of magnitude. It is essential that we managed to incorporate into such coatings also a certain amount of drug. Its slow release into the body is supposed to have analgetic effects during post-surgical period.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Iskra TELA d.d., PE Baterije Zmaj, Šentvid pri Stični, Slovenia: optimisation of battery electrodes;
- BELINKA d.d., Ljubljana, Slovenia: stability of paint suspensions;
- LEK d.d., Ljubljana, Slovenia: composites with controlled release of drugs;
- Predilnica Litija, Slovenia: partner in Nanosciences and Nanotechnologies Centre of Excellence;
- Atotech Podnart, d.d., Slovenia: partner in Nanosciences and Nanotechnologies Centre of Excellence;
- JUB, chemical industry d.d., Dol pri Ljubljani, Slovenia.

POMEMBNI INŠTRUMENTI IN OPREMA

- Vrstični elektronski mikroskop na poljsko emisijo Karl Zeiss Supra 35 VP, opremljen z analizatorjem EDS (Oxford INCA 400);
- sistemi za elektrokemijske, impedančne, mikroimpedančne in električne meritve (EG&G Model 283, Solartron SI 1260, ECI 1286, FRA 1250, HP 4284 LCR meter, Karl Süss, Keithley 237);
- 2 komori Braun za delo v atmosferi z vlago pod 1ppm in vsebnostjo kisika pod 5ppm;
- polielektrolitski titrator (Metrohm, 736 GP Titrino) z detektorjem strujnega toka (Muetek, PCD 03).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Mentorstva:

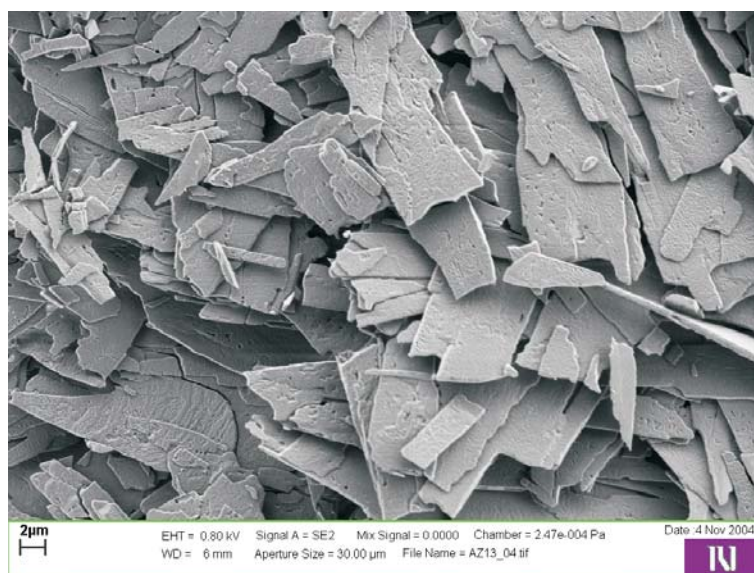
1. ERJAVEC, Boštjan: *Kondenzatorji na osnovi električnega dvo-sloja: tehnologija priprave in karakterizacija*, diplomsko delo, Ljubljana; ŠB. Erjavec, 2006, M. Gaberšček: somentor.

INTERNATIONAL COLLABORATION

- ALISTORE, 6th EU Framework Network of Excellence;
- Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics (FP6-2004-NMP-NI-4) - NANO(BIOPHARMACEUTICS, Integrated project in the 6th EU Framework.

MAJOR EQUIPMENT

- Field-Emission Scanning Electron Microscope (Karl Zeiss Supra 35 VP, equipped with EDS (Oxford INCA 400);
- Systems for electrochemical, impedance, microimpedance and electrical measurements (EG&G Model 283, Solartron SI 1260, ECI 1286, FRA 1250, HP 4284 LCR meter, Karl Süss, Keithley 237);
- 2 Braun dry boxes (humidity < 1ppm, oxygen < 5ppm).



SLIKA 2:

Morfologija naproksena, pripravljena z metodo obarjanja z zamenjavo topila. Tipične dimenzije delcev: 1–10 mikrometrov.

FIGURE 2:

Morphology of naproxen prepared according to a modified precipitation procedure. Typical particle dimensions: 1 – 10 micrometres.

2. GODEC, Aljaž: *Vpliv prostorske restrikcije na nastanek in stabilnost polimorfnih oblik = The influence of space restriction on the formation and stability of polymorphs*. V: VITEZIĆ, Natalija (ur.). 16. simpozij, 27. oktober 2006. 36. Krkine nagrade. Novo mesto: Krka, 2006, M. Gaberšček: mentor.
3. MAVER, Uroš: *Stresalna naprava z modificiranimi polimernimi siti za ločevanje in analizo velikosti delcev = New sieving device with modified polymeric sieves for separation and particle size analysis*. V: VITEZIĆ, Natalija (ur.). 16. simpozij, 27. oktober 2006. 36. Krkine nagrade. Novo mesto: Krka, 2006, str. 75. M. Bele: mentor.

Gostovanja:

- Robert Dominko, Université de Picardie, Amiens, Francija ter Univerza Uppsala, Švedska;
- Janko Jamnik, Max-Planck Institut, Stuttgart, Nemčija.

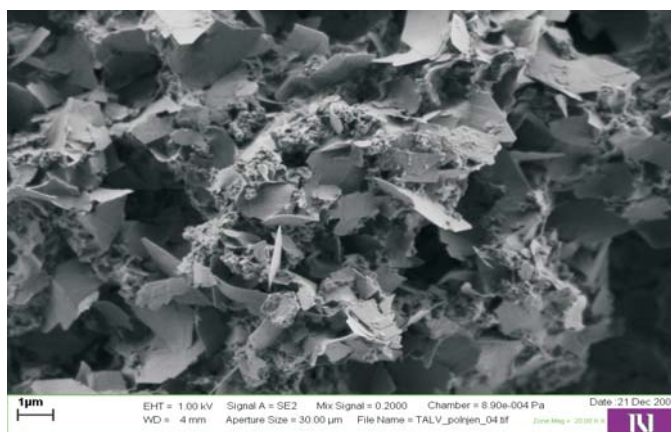
EDUCATION AND IMPORTANT VISITS

Mentorships:

1. ERJAVEC, Boštjan. *Kondenzatorji na osnovi električnega dvo-sloja: tehnologija priprave in karakterizacija : diploma thesis*. Ljubljana: M. Gaberšček: co-mentor.
2. GODEC, Aljaž. The influence of space restriction on the formation and stability of polymorphs. In: VITEZIĆ, Natalija (ed.). 16. symposium, 27. October 2006. (Krka award). Novo mesto: Krka, 2006, M. Gaberšček: mentor.
3. MAVER, Uroš. New sieving device with modified polymeric sieves for separation and particle size analysis. In: VITEZIĆ, Natalija (ed.). 16. symposium, 27. October 2006. (Krka award). Novo mesto: Krka, 2006, p. 75. M. Bele: mentor.

Visits of foreign institutes:

- Robert Dominko, Université de Picardie, Amiens, France and Uppsala University, Sweden.
- Janko Jamnik, Max-Planck Institute, Stuttgart, Germany.



SLIKA 3:

Tanka obloga iz hidroksiapatita za zaščito medicinskih vsadkov. Obloga vsebuje tudi zdravilno učinkovino (drobni delci med ploščami).

FIGURE 3:

Thin hydroxyapatite coating for protection of metallic medical implants. The coating contains a drug substance (seen as powder between the platelets).

L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation



VODJA / HEAD

Prof. dr. Radovan Komel

RAZISKOVALCI / RESEARCHERS

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dr. Marija Anžur-Lasnik (LEK)
dr. Apolonija Bedina Zavec
dr. Irena Fonda
dr. Vladimira Gaberc-Porekar
dr. Katja Galeša
mag. Simona Jevševar (LEK)
dr. Branka Korošec
dr. Nada Kraševc
Menči Kunstelj (LEK)
dr. Ana Lenassi Zupan
dr. Viktor Menart (KI / LEK)

Barbara Podobnik (LEK)
dr. Marjetka Podobnik
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Vanja Smilović
mag. Irena Zore (LEK)

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Gorazd Hribar
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Mateja Kusterle (LEK)
Ljerka Lah
Mateja Novak Štagoj
Špela Peternel
Matjaž Vogelsang

TEHNIČNO OSEBJE / TECHNICAL STAFF

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Karmen Čerkič (LEK)
Ana-Marija Jesenko
Jelka Lenarčič
Nataša Lileg Tašler
Mateja Skok (LEK)
Tea Tomšič



PODROČJA DEJAVNOSTI

Raziskave laboratorija L11 potekajo v okviru združenega programa med Kemijskim inštitutom ter Medicinsko in Veterinarsko fakulteto Univerze v Ljubljani: »Funkcijska genomika in biotehnologija za zdravje« (P1-0104) in treh raziskovalnih projektov: »Mikro in nano delci v biotehnologiji«, »Strukturne raziskave inozitol-polifosfatnih kinaz« (J4-6463) in »Rekombinantno cepivo proti aviarni influenci« (M1-0150).

Raziskovalni program sestavljajo naslednja področja:

- Preučevanje metod za pridobivanje biofarmaceutikov – rekombinantnih citokinov ter njihova modifikacija;
- celična biologija kvasovke *S. cerevisiae*;
- biotehnologija nižjih evkariontov (nitaste glive in kvasovke);
- preučevanje in kloniranje genov za pretvorbe steroidov pri nitastih glivah;
- strukturne raziskave biološko aktivnih molekul;
- funkcijska genomika.

RESEARCH ACTIVITIES

Research work of laboratory L11 is accomplished through a multiparty research programme incorporating National Institute of Chemistry, Faculty of Medicine and Veterinary Faculty of the University of Ljubljana, Slovenia, as well as through three research projects. The research programme is entitled 'Functional genomics and biotechnology for health' (P1-0104) and research projects bear the following titles: 'Micro- and nano-particles in biotechnology' (L4-6171), 'Structural studies of inositol polyphosphate kinases' (J4-6463) and 'Recombinant vaccine against avian flue' (M1-0150).

Research program of Laboratory L11 includes research areas:

- Investigation of approaches to biotechnological production of biopharmaceuticals - recombinant cytokines and their modification.
- Cell biology of the yeast *Saccharomyces cerevisiae*.
- Biotechnology of lower eukaryotes (filamentous fungi and yeasts).

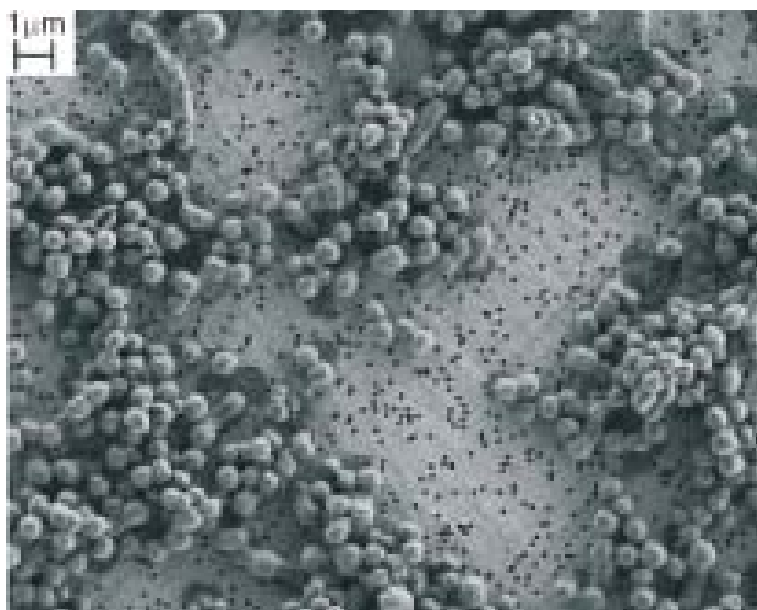
Metodološki pristopi za izvajanje programa so:

- gensko oziroma proteinsko inženirstvo: načrtovanje in pridobivanje novih, delno spremenjenih proteinskih molekul z izboljšanimi lastnostmi za uporabo ali za lažje pridobivanje;
- proteinski laboratorij: modifikacija, izolacija, prečiščevanje in karakterizacija rekombinantnih proteinov;
- fermentacijska tehnologija: preučevanje osnovnih parametrov biosinteze s poudarkom na zakonitostih, ki veljajo za rekombinantne seve;
- celične kulture: gojenje sesalskih celičnih linij; uvajanje novih metod za testiranje biološke aktivnosti biofarmaceutikov;
- funkcijska genomika in proteomika: kvasni dvo-hibridni sistem za ugotavljanje celičnih interakcij "protein-DNA" oz. "protein-protein";

- Study and cloning of steroid bioconverting genes in filamentous fungi.
- Structural studies of biologically active molecules.
- Functional genomics.

Methodological approaches:

- Genetic and protein engineering: design and production of novel, partially modified protein molecules with improved properties for final use or simplified isolation/purification.
- Protein laboratory: isolation, purification and characterisation of recombinant proteins.
- Fermentation technology: studies of basic parameters of biosynthesis, with an emphasis on the principles for recombinant strains.
- Cell cultures: cultivation of mammalian cell lines; introduction of new methods for biological activity testing of cytokines.



SLIKA 1:

Neklasična inkluzijska telesa GCSF iz *E. coli*, pridobljena s homogeniziranjem celic in pazljivim spiranjem z destilirano vodo. Slikano z elektronskim mikroskopom, na z zlatom prevlečeni polikarbonatni podlogi Isopore™

FIGURE 1:

Non-classical inclusion bodies of GCSF from *E. coli*, prepared by cell disruption in a homogenizer and thoroughly washed in pure water, as observed under scanning electron microscope on a gold-coated polycarbonate Isopore™ membrane filter.

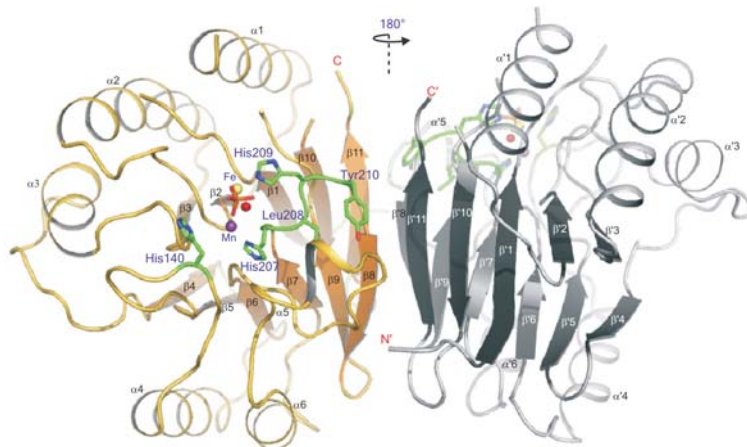
- funkcijska analiza onkogenih mutacij v kvasovkah;
 - lokalizacija celičnih proteinov s fluorescenčno mikroskopijo;
 - pretočna citometrija in sortiranje celic;
 - preučevanje tri-dimenzionalnih struktur biološko aktivnih molekul z X-žarkovno kristalografijo in nuklearno magnetno resonanco (NMR).
- Genomics and proteomics: yeast two-hybrid system at looking for cellular "protein-DNA" and "protein-protein" interactions; functional analysis of human oncogenic mutations in yeast.
 - Protein cellular localisation by fluorescence microscopy.
 - Flow cytometry and cell sorting.
 - Three-dimensional structure determination of biologically active molecules by X-ray crystallography and nuclear magnetic resonance (NMR).

BIBLIOGRAFIJA

- 11 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 2 kratka znanstvena prispevka
- 3 poljudni članki
- 9 intervjujev
- 1 srednješolski, osnovnošolski ali drugi učbenik z recenzijo
- 1 priročnik, slovar, leksikon, atlas, zemljevid

BIBLIOGRAPHY

- 11 Original Scientific Articles
- 1 Review Article
- 2 Short Scientific Articles
- 3 Popular Articles
- 9 Interviews



SLIKA 2:

Dimer Rv0805 (protomera vsebujeta aminokislino 1-278). Protomera Rv0805¹⁻²⁷⁸ (rumeno in sivo) dimerizirata tako, da sta aktivni mesti na nasprotnih straneh dimera. Kovinski ioni so označeni z barvastimi kroglicami, fosfat (P, oranžno; O, rdeče), pomembne aminokislino blizu stika med molekulama pa kot paličice (C, zeleno; N, modro; O, rdeče). Planarna voda je označena kot rdeča kroglica. Dvoštevna kristalografska os je označena s prekinjeno črto.

FIGURE 2:

The Rv0805 dimer (of protomers containing amino acids 1-278). Rv0805¹⁻²⁷⁸ protomers (yellow and grey) dimerize in a manner that places one active site on each side of the dimer. Metals are represented by labeled spheres and phosphate (P, orange; O, red) and residues proximal to the dimer interface by sticks (C, green; N, blue; O, red). The planar water is rendered as a red sphere. The two-fold crystallographic axis is marked by a dotted line.

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|----|---|----|--|
| 2 | objavljena znanstvena prispevka na konferencah | 1 | Reviewed Secondary and Primary School Textbook or Other Textbook |
| 10 | objavljenih povzetkov znanstvenih prispevkov na konferencah | 1 | Manual, Dictionary, Lexicon, Atlas, Map |
| 1 | objavljeni povzetek strokovnega prispevka na konferenci | 2 | Published Scientific Conference Contributions |
| 1 | patentna prijava | 10 | Published Scientific Conference Contribution Abstracts |
| 1 | patent | 1 | Published Professional Conference Contribution Abstract |
| 1 | prispevek na konferenci brez natisa | 1 | Patent Application |
| 4 | vabljeni predavanja na konferencah brez natisa | 1 | Patent |
| 5 | diplom | 1 | Unpublished Conference Contribution |
| 1 | magisterij | 4 | Unpublished Invited Conference Lectures |
| 2 | doktorata | 5 | Undergraduate Theses |
| 2 | uredništvu revij | 1 | Master's Thesis |
| | | 2 | Doctoral Dissertations |
| | | 2 | Journal Editorships |

DOSEŽKI V LETU 2006

V sklopu raziskav **biosinteze rekombinantnih proteinov** (biofarmaceutikov) smo raziskovali procese, ki v bakteriji *E. coli* vodijo do tvorbe »neklasičnih«
inkluzijskih teles. Njihova značilnost je, da vsebujejo visok delež pravilno zvitega tarčnega proteina oziroma njegovega prekursorja, ki ga lahko iz inkluzijskih teles izoliramo z blago ekstrakcijo pri nedena-
turirajočih pogojih. Postopek izolacije se tako bistveno skrajša, poceni in postane okolju
prijaznejši, kar je za biotehnoške postopke zelo pomembno.

Neklasična inkluzijska telesa so zanimiva tudi zaradi nekaterih zanimivih lastnosti (poroznost, krčenje pri nizkem pH), ki zmanjšajo ekstra-
ktabilnost tarčnega proteina in tako vplivajo na proces izolacije. Raziskave (*in vivo* ter *in vitro*) kažejo, da proteini v inkluzijskih telesih niso zaščiteni pred encimsko razgradnjo. Prav te lastnosti neklasičnih inkluzijskih teles so pomembne pri nadaljnjih raziskavah, saj odkritje lahko uporabimo tako v biotehnologiji kot v medicini (konformacijske bolezni).

Kemijski inštitut je eden od partnerjev v mednarodnem evropskem projektu z naslovom »Nanoscale Functionalities for Targeted Drug Delivery of Biopharmaceutics«
ali krajše »Nanobiopharmaceutics«, ki teče v sklopu 6. okvirnega programa EU (FW6) od leta 2006 do

RESULTS IN 2006

Biosynthesis of recombinant proteins in bacteria *E. coli* at low temperatures leads to the formation of "nonclassical" inclusion bodies (nclBs). They contain high amount of properly folded target protein (or its precursor), which can be easily extracted from nclBs with mild extraction in non-denaturing conditions. This results in much shorter, cheaper and environment-friendly downstream process.

"Nonclassical" inclusion bodies have some interesting properties (porosity, low pH contractibility) that reduce extractability of target protein from nclBs and thus affect downstream process. Studies show that proteins inside nclBs are not protected from proteolysis neither inside bacterial cells nor after the isolation. We believe the phenomenon of nclBs is worth studying further as important implications in biotechnology and medicine are foreseen.

National Institute of Chemistry is one of the partners in an international European project "Nanoscale Functionalities for Targeted Drug Delivery of Biopharmaceutics" (2006-2009) or shortly "Nanobiopharmaceutics", within the Sixth Framework Programme for research and technological development (FP6). Laboratories L07, L10 and L11 are engaged in this research.

2009, pri njem pa sodelujejo oddelki L07, L10 in L11. Namen tega projekta je uporabiti naravno lastnost proteinskih molekul, da težijo k agregaciji oz. samozdruževanju, vendar bomo uporabili proteinske analoge s posebnimi podaljškimi, ki bodo sposobni nadzorovane agregacije proteinskih molekul v proteinske nanostrukture. Kot modelne proteine bomo uporabili analoge dejavnika tumorske nekroze alfa (TNF-alfa). Te **proteinske nanostrukture** bi lahko služile kot osnova za protitumorsko terapijo s podaljšanim delovanjem ali pa za sprožitev povečanega imunskega odziva in s tem nastanka protiteles proti TNF-alfa, katerega raven je pri kroničnih vnetnih stanjih, kot so revmatoidni artritis, Chronova bolezen in psoriza, zelo povišan.

V letu 2006 smo s pomočjo kovinsko kelatne afinitetne kromatografije (IMAC) izolirali večjo količino proteina His10-TNF (50 mg) in ga okarakterizirali. Naredili smo tudi nekaj preliminarnih poskusov agregacije analoga His10-TNF s kovinskimi ioni in polifunkcionalnimi kelatorskimi molekulami.

Ena izmed glavnih ovir za širšo terapevtsko uporabnost TNF- α je prav gotovo njegova sistemska toksičnost ter kratkoživost pri aplikacijah *in vivo*. **Kemijska modifikacija proteinov** s polietilenglikolom (PEG) bi lahko predstavljala dobro rešitev, saj je znano, da pegilacija podaljša čas kroženja farmacevtsko uporabljenih proteinov v organizmu, zviša stabilnost proteinov in doprinese k zmanjšanju imunogenosti. Najbolj razširjen pristop modifikacije proteinov s PEG-om je naključna pegilacija, ki je usmerjena na ϵ -amino skupine lizinov ter na N-terminalno amino skupino. Ker je število dostopnih Lys na proteinu ponavadi veliko, nastane zelo kompleksna zmes pozicijskih izomerov in multipegiliranih proteinov. Za bolj specifično pegilacijo smo preizkusili pristop pegilacije na afinitetni koloni z imobiliziranimi kovinskimi ioni (IMAC), na katero smo vezali analog TNF- α z oznako LK-801, ki vsebuje dve histidinski mutaciji. Zaradi trimerne strukture nastane klaster šestih

The aim of the project is to exploit the natural propensity of protein molecules, which tend to self-assemble into higher structures, however, specifically designed protein analogues with special tags enabling controlled aggregation and **protein nanostructure** formation will be employed. Specifically designed analogues of tumor necrosis factor alpha (TNF-alpha) will serve as model proteins. Such protein nanostructures could be used in anti-cancer therapy enabling sustained release of captured protein or for the activation of immune response and generation of antibodies against TNF-alpha that is pathogenically elevated in various chronic diseases (rheumatoid arthritis, Crohn disease, psoriasis, etc.)

The project started in October 2006 by preparation and characterisation of a larger amount of His10-TNF (50 mg). Some preliminary tests of aggregating His10-TNF with metal ions and polyfunctional biocompatible chelating compounds were also performed.

Major limitations for broad therapeutic applicability of tumor necrosis factor alpha (TNF- α) are severe systemic toxicity and very short *in vivo* half-life. Taking into account that today widely used **chemical modification of proteins** by polyethylene glycol (PEG) generally increases *in vivo* circulating half-life, improves protein stability and reduces immunogenicity, pegylation might be an appropriate solution. The most commonly performed pegylation reaction is random pegylation targeted preferentially towards ϵ -amino groups of lysines (Lys) and the N-terminal amino group. Usually, the number of surface exposed Lys residues is high leading to complex mixtures of numerous positional isomers and multi-pegylated forms. To reduce the number of different pegylated species an on-column pegylation approach was tested using Immobilized Metal Affinity Chromatography (IMAC). TNF- α analogue LK-801 with double histidine mutation was used as a model protein. Due to the trimeric structure, LK-801 possesses a surface cluster of six histidines enabling excellent chromatographic

histidinov, ki omogoča odlično vezavo na različnih nosilcih IMAC. Primerjali smo selektivnost in stopnjo pegilacije modelnega proteina pri reakciji na koloni oz. v raztopini ter preizkusili izolacijo in pegilacijo LK-801 v eni stopnji. Rezultati kažejo, da IMAC ne ponuja samo možnosti učinkovite pegilacije na koloni, temveč tudi perspektivo za sklopljen proces čiščenja rekombinantnega proteina in pegilacije v imobilizirani obliki na koloni.

V sklopu raziskav **humanega limfotoksina alfa (LT- α)** smo izdelali strategijo za izolacijo podaljšane oblike rekombinantnega LT- α . Uporabili smo rekombinantni sev bakterije *E. coli*, ki izraža humani LT- α s histidinskim podaljškom (His7) na N-terminalnem koncu molekule. Večina rekombinantnega proteina se je izločala v obliki inkluzijskih teles. Ker so predhodni poskusi pokazali, da ne gre za »neklasična« inkluzijska telesa, smo le-ta raztopili v visoki koncentraciji denaturanta. Protein smo v denaturirani obliki vezali na kromatografski nosilec Ni-NTA, ki specifično veže proteine s številnimi zaporednimi histidinskimi ostanki. Elucijo smo izvedli s pufrom, ki je vseboval EDTA. Renaturacijo denaturiranega proteina smo izvedli z zamenjavo pufru, redčenjem v renaturacijskem pufru in renaturacijo na koloni. Najboljše rezultate smo dosegli z redčenjem v pufru, ki je vseboval 2 M ureo in 1 M nemicelarni sulfobetain NDSB 201. V sodelovanju z National Institute for Biological Standards and Control iz Velike Britanije smo objavili študijo o **in vitro** biološki aktivnosti interferona alfa. Svetovna zdravstvena organizacija zahteva, da so mednarodni biološki standardi dolgoročno stabilni pri priporočeni temperaturi hranjenja. Toplotna stabilnost se običajno ocenjuje v študijah s pospešeno toplotno razgradnjo, pri čemer ampule liofiliziranega standarda pred testiranjem shranjujemo pri povišanih temperaturah. Za potrditev predvidene visoke toplotne stabilnosti, drugega mednarodnega standarda za interferon alfa-2b (IFN- α 2b; 95/566), smo preverili aktivnost ampuliranih vsebin tega standarda po

behaviour and specific orientation of the molecule. Additionally to on-column pegylation of the purified LK-801, a coupled process of protein purification and on-column pegylation was tested. Our results suggest that IMAC offers not only the possibility of an efficient on-column pegylation but also the prospect of the coupled purification and on-column pegylation processes.

In the framework of recombinant **human lymphotoxin alpha (LT- α)** studies, a strategy for isolation of the extended form of LT- α was developed. For biosynthesis, a previously prepared *E. coli* strain capable of expressing human LT- α with a histidine tag (His7) appended to the natural hydrophobic N-terminus was used. Majority of the expressed recombinant protein was found in the form of inclusion bodies; however the preliminary experiments denied their »non-classical« nature, therefore solubilization was performed with high concentrations of denaturants. Completely denatured protein was purified on the Ni-NTA matrix, which selectively binds proteins with numerous adjacent histidine residues. After purification, various types of renaturation were tested. On-column renaturation was also performed, however, the highest recovery of the active protein was obtained by dilution with renaturation buffer containing 2 M urea and 1 M NDSB 201.

In cooperation with National Institute for Biological Standards and Control we published study on **in vitro** testing of biological activity of interferon alpha. A World Health Organization requirement for biological standards is that they should exhibit long-term stability at their recommended storage temperature. Thermal stability is usually evaluated in accelerated thermal degradation studies, where ampoules of the lyophilized standard are stored at elevated temperatures before testing. To confirm the predicted very high thermal stability of the 2nd international standard of human interferon alpha-2b (IFN- α 2b; 95/566), we tested the potency of the ampouled contents

9 letih hrambe pri temperaturah med -150°C in 56°C . Glede na visoko variabilnost znotraj poskusa pri testu protivirusne aktivnosti (AVA), smo preučevali nov pristop testiranja z reporterskim genom (RGA), ki temelji na vzbujanju izločanja alkalne fosfataze (SEAP), za primerjavo in točnost ocen aktivnosti. Pokazali smo, da je RGA podal podobne ocene ob skupni nižji variabilnosti. Poleg tega je pretvorbo p-nitrophenyl fosfata s SEAP v rumeno obarvani produkt moč spremljati kinetično. Pokazali smo, da so odčitki absorbance naraščali s časom v odvisnosti od naraščajoče koncentracije interferona. Ko so bili od časa odvisni prirastki izrisani grafično, so bili nakloni premic sorazmerni z uporabljenimi koncentracijami. Ta pristop je omogočil uporabo posamezne redčitve vzorcev interferona za oceno njegove aktivnosti z interpolacijo na standardno premico pod pogojem molekularne strukturne identičnosti s standardom. Pristop se zdi privlačen za visoko pretočno testiranje aktivnosti različnih R&D vzorcev interferona in morebiti širše tudi drugih citokinov.

Mejoza je evolucijsko ohranjen proces, pri katerem nastanejo haploidne spore ali spolne celice. Za normalno raven sporulacije in preživetje spor v kvasovki *Saccharomyces cerevisiae* je potreben protein Ecm11. Ta protein ima vlogo v zgodnjih fazah mejoze, kjer je njegova funkcija vezana na podvojevanje DNA in crossing-over. Znano je, da se v dvo-hibridnem sistemu Ecm11 veže na protein SUMO (Smt3). Poškodbe uravnavanja sistema SUMO pri človeku povzročijo tumorigenezo, spremenjen vnetni odziv in nevrodegenerativne bolezni. Zato je zelo pomembno, da razumemo proces sumoilacije, da odkrijemo kateri proteini so uravnavani s proteinom SUMO in ugotovimo delovanje njihove sumoilacije. V letu 2006 smo se osredotočili na preučevanje uravnavanja Ecm11 s proteinom SUMO. Sumoilacijo Ecm11 smo potrdili s pomočjo koimunoprecipitacije. Za ugotavljanje biološke vloge sumoilacije tega proteina med mejozo smo mu z mutacijami spremenili predvidena vezavna mesta za SUMO.

of this standard after 9 years storage at temperatures ranging from -150°C to 56°C . Since IFN- $\alpha 2\text{b}$ potency estimates derived from the results of antiviral assays (AVA) showed high within assay variability, we investigated a novel reporter gene assay (RGA) based on induction of secreted alkaline phosphatase (SEAP) for comparability and precision of such estimations. We showed that this RGA generated comparable estimates with overall lower variation. Additionally, the SEAP conversion of p-nitrophenyl phosphate to yellow product could be followed kinetically. Absorbance readings were shown to increase with time in proportion with increasing concentration of IFN. When the time-dependent increments of absorbance were plotted graphically, the slopes of lines corresponded to concentration. This approach enabled single dilutions of IFN samples, identical in molecular structure to an IFN standard, to be used for potency estimates by interpolation of slope value against those of the standard at fixed concentrations. It appears attractive for high through-put potency testing of various R&D IFN samples, and potentially has wider applicability to other cytokine determinations.

Meiosis is evolutionally conserved process, which is required to haploidize the genome prior to spore or gamete formation. Protein Ecm11 is necessary for the proper level of sporulation and spore viability in the yeast *Saccharomyces cerevisiae*. It is required in early stages of meiosis where its function is related to DNA replication and crossing-over. From previous study it is known that Ecm11 interacts with protein SUMO (Smt3) in the two-hybrid system. Damaged regulation of the SUMO system contributes to human tumorigenesis, abnormal inflammatory response, and neurodegenerative diseases; therefore, it is very important to understand the process of sumoylation, to identify the SUMO targets, and to determine the function of their sumoylation. In the year 2006 we focused on modification of Ecm11 by SUMO. We were able to confirm the sumoylation of Ecm11 by coimmunoprecipitation. To

S pomočjo mutant smo določili specifično mesto sumoilacije Ecm11 na Lys5 in pokazali, da sumoilacija na Lys5 direktno uravnava delovanje Ecm11 v mejozi. Po drugi strani pa sumoilacija Ecm11 ne vpliva na vlogo proteina v vegetativnem celičnem ciklu. S pomočjo dvo-hibridnega sistema smo pokazali, da Ecm11 interagira s SUMO ligazo Siz2, vendar Siz2 ni nujno potrebna za njegovo sumoilacijo. Siz2 je verjetno glavna SUMO ligaza za Ecm11, vendar jo ob odsotnosti lahko nadomesti druga SUMO ligaza, najverjetneje Siz1.

Kvasovka *Saccharomyces cerevisiae* je kot najpreprostejši evkariont uporabna tudi za študije biokemije številnih človeških bolezni. Tako smo z uporabo *S. cerevisiae* preučevali delovanje človeškega DNA popravljalnega mehanizma (MMR – DNA mismatch repair), ki lahko ob nedelovanju privede do nastanka raka. Razvili smo **kvasni model za preučevanje vpliva polimorfizma človeških MMR-genov** na funkcijo MMR mehanizma v celici. S tem smo omogočili razločevanje tistih genskih različic, ki vplivajo na funkcijo MMR mehanizma, od tistih, ki na MMR-funkcijo ne vplivajo. To je pomembno za učinkovito napoved nagnjenosti k rakavemu obolenju in pravilno izbiro terapije obolelih za rakom.

V sklopu preučevanja **citokromov P450** nitaste glive *Cochliobolus lunatus* smo pripravili več mutant z utišanimi geni za različne proteine in jih potrdili. S preučevanjem katalitskih značilnosti benzoatne para-hidroksilaze (BPH) smo dokazali, da so naravna fenolna protiglivna sredstva inhibitorji BPH. Skupaj z benzoatom povečajo učinek protiglivnega delovanja. Nekateri rezultati kažejo, da je BPH pomembna ne samo pri detoksifikaciji benzoata, temveč tudi omenjenih naravnih protiglivnih učinkovin, saj je mutanta z utišanim genom BPH v njihovi prisotnosti izkazala večjo inhibicijo rasti. Verjetno je katalitska funkcija BPH poleg hidroksilacije še demetilacija. Utišali smo tudi gen za verjetno epoksidno hidrolazo in citokrom P450 reduktazo (CPR2). Nobeden od omenjenih

observe biological role of sumoylation of Ecm11 during meiosis we mutated predicted SUMO consensus sites in Ecm11. Using these mutant strains we identified a specific site of sumoylation in Ecm11 at Lys5 and provided evidence that sumoylation at this site directly regulates Ecm11 function in meiosis. On the other hand, no relationship was observed between sumoylation of Ecm11 and its role in the vegetative cell cycle. We showed that Ecm11 interacts with Siz2 SUMO ligase in the two-hybrid system; although Siz2 is not essential for the Ecm11 sumoylation. Siz2 is probably the major ligase for Ecm11 protein, but could be replaced by some other SUMO ligase, most probably Siz1. Yeast *Saccharomyces cerevisiae* is one of the simplest eukaryote, also used for biochemical studies of various human diseases. Using yeast cells we studied human mismatch repair (MMR) function, which if impaired can lead to cancerogenesis. We developed a novel approach for **functional characterization of human polymorphic MMR genes** in yeast that enables pathogenic *MLH1* variants to be discriminated from polymorphisms that have no effect on MMR function. This is essential, not only for effective diagnosis of cancer predisposition, but also for choosing the appropriate chemotherapy for cancer patients.

In the scope of research of **cytochromes P450** of *Cochliobolus lunatus* several deletion mutants of different proteins were prepared. Further analyses of catalytic properties of benzoate para hydroxylase (BPH) showed that naturally occurring phenolic antifungal substances behave as competitive inhibitors of BPH. If the fungi were grown in the presence of phenolic antifungal substances and benzoate, increased growth inhibition was observed. Some of the results lead to the conclusion that BPH is not only an important enzyme in detoxification of benzoate, but has also a role in detoxification of natural antifungal substances. Deletion mutants of putative epoxide hydrolase and cytochrome P450 reductase 2 (CPR2) were constructed and none of the above proteins was

proteinov za glivo ni esencionalen. Da bi ugotovili funkcije proteinov, smo v bakteriji *E. coli* izrazili gen za CPR2, v teku pa je kloniranje gena za CPR1 in gena za 14-alfa demetilazo iz glive *C. lunatus*. Z degenerativnimi začetnimi oligonukleotidi iščemo morebitni drugi gen za 14-alfa demetilazo. Iz cDNA skušamo pomnožiti in pridobiti tudi druge gene za citokrome P450 z neznanimi funkcijami. Uspešno smo izrazili še ne opredeljeni citokrom P450 iz glive rodu *Aspergillus*, za katerega na podlagi bioinformatičkih analiz domnevamo, da sodeluje pri hidroksilaciji steroidov. V teku je njegova funkcijska karakterizacija. Naredili smo bioinformatičke analize P450-omov 36 v celoti znanih glivnih genomov in ugotovili, da obstaja korelacija med velikostjo P450-oma in številom relevantnih reduktaz. Podrobneje smo analizirali filogenetske povezave med CPR in drugimi prisotnimi reduktazami v anotiranih glivnih genomih.

Na projektu **inozitol polifosfatnih kinaz ter inozitol polifosfatov**, ki so pomembni dejavniki pri prenosu signalov v živi naravi, smo v letu 2006 nadaljevali z biokemijskimi in strukturnimi raziskavami encima inozitol heksakisfosfatna kinaza ter polifosfatnih derivatov inozitola, ki jih ta encim sintetizira. Uspeli smo optimizirati pogoje encimske reakcije za čim večji izkoristek nastanka produktov, katerih strukturo smo nato preučevali z uporabo prilagojenih metod ICP-MS, LC-MS in NMR. Uspeli smo dešifrirati že večino produktov tega encima.

Pri preučevanju **metabolizma cikličnih nukleotidov**, pomembnih sekundarnih sporočevalnih molekul, smo v letu 2006 uspešno nadaljevali strukturne in biokemijske raziskave fosfodiesteraze Rv0805 iz *Mycobacterium tuberculosis*. Rv0805 je do sedaj edina znana fosfodiesteraza v genomu te patogene bakterije, ki razgrajuje ciklične nukleotide (cAMP in cGMP). Po strukturi se zelo razlikuje od evkariontskih encimov s podobnimi funkcijami. Pokazali smo, da je Rv0805 dimeren encim, v katerega aktivnem mestu sta vezana

proven essential for the fungus. Functional cloning of different *C. lunatus* genes in *E. coli*, such as CPR2 (already expressed), CPR1 and 14-alfa demethylase, is in progress. Attempts to find a probable second gene with the 14-alfa demethylase activity using degenerative primers are going on as well as experiments for amplification of other cytochrome P450 genes with unknown function which will be expressed in *E. coli*. In addition, a cytochrome P450 of unknown function from *Aspergillus sp.*, which is according to bioinformatic analysis involved in hydroxylation of steroids, was already expressed and its functional characterization is in experimental procedure. Bioinformatic analysis of cytochromes P450 from 36 fungi with sequenced genomes was performed and it was found that there is a correlation between the number of cytochromes P450 in the organism and the number of relevant reductases. And finally, analysis of phylogenetic correlation between CPR and other reductases, with the help of annotated fungal genomes, was completed. In 2006 we have achieved a major step forward in the studies of **the inositol hexakisphosphate kinase and its products**, inositol polyphosphates, containing energy rich pyrophosphate bonds. Enzymatic assays were optimized to achieve high yields of the polyphosphorylated products, which have been used in further studies. Using specifically adapted methods for ICP-MS, LC-MS and NMR, we have been able to decipher the structures of most of the energetically rich molecules which are synthesized by the inositol hexakisphosphate kinase.

Cyclic nucleotide monophosphate (cNMP) hydrolysis in bacteria and eukaryotes is brought about by distinct cNMP phosphodiesterases (PDEs). Since these enzymes differ in amino acid sequence and properties, they have evolved by convergent evolution. Cyclic NMP PDEs cleave cNMPs to NMPs, and the Rv0805 gene product is, to date, the only identifiable cNMP PDE in the genome of *Mycobacterium tuberculosis*. We have earlier shown that

kovinska iona Fe^{3+} in Mn^{2+} . Mutacijske analize so pokazale, da sta kovini v aktivnem mestu koordinirani z evolucijsko ohranjenimi aminokislinami, kot so aspartat, histidin in asparagin. Določili smo kristalno strukturo katalitične domene encima Rv0805, ki je soroden kalcineurin-podobnim fosfatazam. Iz kristalne strukture je razvidno, da sta ravno kovinska iona v aktivnem mestu pomembna za dimerizacijo proteina in tako igrata tako strukturno kot katalitično vlogo. Določili smo tudi kristalno strukturo dveh mutant Rv0805, mutante Asn97Ala, kjer je mutirana aminokislina, ki koordinira Mn^{2+} , ter mutante Asp66Ala, ki zaradi te mutacije izgubi katalitično aktivnost za naravni substrat cAMP. Obe strukturi pomembno prispevata k boljšemu razumevanju katalitičnih lastnosti tega encima. V aktivnem mestu strukture divjega tipa Rv0805 je v bližini kovinskih ionov vezan fosfatni ion, v primeru mutante Asp66Ala pa je na tem mestu vezan kakodilatni ion. Unikatno vezavno mesto substrata v aktivnem mestu Rv0805 smo določili s pomočjo računalniških simulacij in tako odkrili potencialno vlogo His140 pri vezavi cAMP, kar smo kasneje tudi prikazali z mutacijsko analizo. Tako ta prva opisana kristalna struktura bakterijske fosfodiesteraze, ki razgrajuje ciklične nukleotide, znatno prispeva k boljšemu razumevanju hidrolize cAMP s tipom fosfodiesteraz razreda III, v katerega spada tudi Rv0805.

Od junija 2006 teče v okviru Ciljnega raziskovalnega programa »Znanje za varnost in mir« projekt z naslovom »Rekombinantno cepivo proti aviarni influenci«. Namen projekta je uporabiti metilotrofno kvasovko *Pichia pastoris* kot gostiteljski sistem za izražanje plaščnih proteinov virusa aviarne influence, proteine izolirati in uporabiti za imunizacijo piščancev. V prvi stopnji smo pripravili seve kvasovke *Pichia pastoris* z različnimi genskimi konstrukti in dokazali izražanje rekombinantnih virusnih proteinov.

Rv0805 is a cAMP/cGMP dual specificity PDE, and is unrelated in amino acid sequence to the mammalian cNMP PDEs. Rv0805 is a dimeric, Fe^{3+} - Mn^{2+} binuclear PDE, and mutational analysis demonstrated that the active site metals are co-ordinated by conserved aspartate, histidine and asparagine residues. We determined the crystal structure of the catalytic core of Rv0805 which is distantly related to the calcineurin-like phosphatases. The structure of the Rv0805 dimer shows that the active site metals contribute to dimerization and thus play an additional structural role apart from their involvement in catalysis. We also solved the crystal structures of the Asn97Ala mutant protein that lacks one of the Mn^{2+} co-ordinating residues as well as the Asp66Ala mutant that has a compromised cAMP hydrolytic activity, providing a structural basis for the catalytic properties of these mutant proteins. A molecule of phosphate is bound in a bidentate manner at the active site of the Rv0805 wild-type protein, and cacodylate occupies a similar position in the crystal structure of the Asp66Ala mutant protein. A unique substrate binding pocket in Rv0805 was identified by computational docking studies, and the role of the His140 residue in interacting with cAMP was validated through mutational analysis. This report on the first structure of a bacterial cNMP PDE thus significantly extends our molecular understanding of cAMP hydrolysis in class III PDEs.

In June 2006 we started a research project »Recombinant vaccine against avian flu«, which is a part of the Target Research Programme entitled »Knowledge for safety and peace«. The aim of this project is to employ the methylotrophic yeast *Pichia pastoris* as the host system for expressing coat proteins of the avian influenza virus, to isolate the recombinant proteins and utilise them for immunisation of chickens. In the first phase, using various gene constructs, several recombinant strains of *Pichia pastoris* were created and expression of the recombinant viral proteins confirmed.

SODELOVANJE Z INDUSTRIJO

- Laboratorij združuje raziskovalce Kemijskega inštituta in Lek-a d.d., Biofarmacevtika, tako da gre za mešano skupino, ki že vrsto let deluje na skupnih raziskovalnih projektih.

MEDNARODNO SODELOVANJE.

- FW6-2004-NMP-NI-4; IP 026723-2 NANO-BIOPHARMACEUTICALS: Integrated FW6 Project "Nanotechnology-based Targeted Drug Delivery" (V. Gaberc-Porekar, V. Menart – partnerstvo pri projektu; 2006–2009).
- MIRG-6-CT-2005-014882: EC Marie Curie International Reintegration Grant "Structural Studies of Inositol poly-Phosphate Kinases" (M. Podobnik; 2005–2007).
- ICGEB CSA (International Centre for Genetic Engineering and Biotechnology): R. Komel – član Znanstvenega sveta ICGEB (CSA – Council of Scientific Advisers; drugi mandat 2007–2009).
- EC mreža odličnosti NANOFUN-POLY (V. Menart, V. Gaberc-Porekar – članstvo v mreži odličnosti; 2004–2007).
- Indian Institute of Science, Bangalore, Indija: sodelovanje s prof. Sandhya Visweswariah na projektu "Strukturne študije cAMP-fosfodiesteraze iz *M.tuberculosis*" (M. Podobnik).
- Johns Hopkins University Medical School, Baltimore, USA: sodelovanje z dr. Rashina Bhandari iz laboratorija prof. Solomona Snyderja na projektu "Strukturne raziskave inozitol polifosfatnih kinaz" (M. Podobnik).

POMEMBNEJŠI INSTRUMENTI IN DRUGA OPREMA

- Laboratorij za gensko tehnologijo,
- laboratorij za izolacijo, čiščenje in karakterizacijo (rekombinantnih) proteinov,
- laboratorij za celične kulture,
- mikrobiološki laboratorij,
- laboratorij z bioreaktorji.

Vsi omenjeni laboratoriji so ustrezno opremljeni

COLLABORATION WITH INDUSTRY

- Laboratory L11 represents a research group composed of researchers from the National Institute of Chemistry (NIC) and the Pharmaceutical Company Lek, d.d., Biopharmaceuticals, Slovenia, which work together on selected research projects.

- MIRG-6-CT-2005-014882: EC Marie Curie International Reintegration Grant "Structural Studies of Inositol poly-Phosphate Kinases" (M. Podobnik; 2005 - 2007).

INTERNATIONAL COLLABORATION

- FW6-2004-NMP-NI-4; IP 026723-2 NANO-BIOPHARMACEUTICALS: Integrated FW6 Project "Nanotechnology-based Targeted Drug Delivery" (V. Gaberc-Porekar, V. Menart – project partnership; 2005/06 - 2008/09).

- MIRG-6-CT-2005-014882: EC Marie Curie International Reintegration Grant "Structural Studies of Inositol poly-Phosphate Kinases" (M. Podobnik; 2005 - 2007).

- ICGEB CSA (International Centre for Genetic Engineering and Biotechnology): R.Komel – CSA Member (CSA – ICGEB Council of Scientific Advisers; 1st mandate, 2004 - 2007).

- EC Network of Excellence NANOFUN-POLY (V. Menart, V. Gaberc-Porekar – membership in; 2004 - 2007).

- Indian Institute of Science, Bangalore, Indija: collaboration with Prof. Sandhya Visweswariah; project "Structural Studies of cAMP-phosphodiesterase from *M.tuberculosis*" (M. Podobnik).

- Johns Hopkins University Medical School, Baltimore, U.S.A.: collaboration with Dr. Rashina Bhandari from the laboratory of Prof. Solomon Snyder on the "Structural studies of inositol poly-phosphate kinases" project (M. Podobnik).

IMPORTANT INSTRUMENTS AND OTHER EQUIPMENT

- Laboratory for gene technology

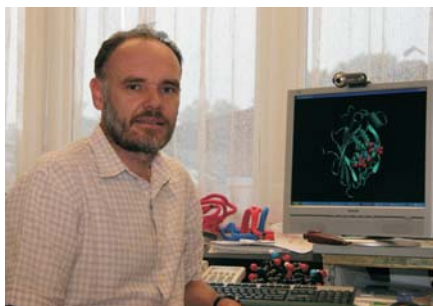
za izvajanje navedenih projektov, kot pomembnejše pa posebej navajamo naslednjo opremo:

- pretočni citometer z možnostjo sortiranja celic (Beckman Coulter),
 - fluorescenčni mikroskop (Zeiss) s sistemom za slikanje,
 - stereo mikroskop (Nikon),
 - fluorimeter (PTI),
 - 2 UV/VIS spektrofotometra (Agilent, Hewlett-Packard),
 - Chirascan CD Spectrometer (Applied Photo-physics, konzorcij),
 - Dynamic Light Scattering Detector (DynaPro),
 - ProExpress Imaging System za denzitometrično obdelavo (Perkin Elmer),
 - Isothermal Titration Calorimeter (MicroCal, konzorcij),
 - 4 preparativni sistemi za kromatografske separacije proteinov (Amersham Biosciences, Knauer),
 - 1 analitski HPLC sistem (Waters),
 - 2 računalniško vodena laboratorijska bioreaktorja (Applikon),
 - 2 sistema za pripravo Milli-Q vode (Millipore),
 - hladilne kapacitete +4°C, -20°C in -70°C,
 - 4 stresalniki,
 - sklop aparatov za pomnoževanje in sekvenčno analizo DNA,
 - sistem za dokumentacijo gelov (Chemi Doc, BIO-RAD).
- Laboratory for isolation, purification and characterisation of (recombinant) proteins
 - Laboratory for cell cultures
 - Laboratory for microbiology
 - Laboratory with bio-reactors
- Laboratories are equipped with modern instruments for the realization of the above mentioned projects. This is a list of more significant instruments:
- Flow cytometer with cell sorter (Beckman Coulter)
 - Fluorescence microscope with CD camera (Zeiss)
 - Stereo microscope (Nikon)
 - Fluorimeter (PTI)
 - 2 UV/VIS spectrophotometers (Agilent, Hewlett-Packard)
 - Chirascan CD Spectrometer (Applied Photo-physics, consortium)
 - Dynamic Light Scattering Detector (DynaPro)
 - ProExpress Imaging System for densitometric analysis (Perkin Elmer)
 - Isothermal Titration Calorimeter (MicroCal)
 - 4 preparative HPLC systems for protein separations (Amersham Biosciences, Knauer)
 - Analytical HPLC system (Waters)
 - 2 computer assisted laboratory bio-reactors (Applikon)
 - 2 systems for Milli-Q water (Millipore)
 - Cooling and freezing capacities (+4°C, -20°C and -70°C)
 - Gel documentation system (Chemi-Doc, BIO-RAD)
 - Shakers and Incubators
 - Set of instruments for PCR and DNA sequence analysis.

L12

Laboratorij za biotehnologijo

Laboratory of Biotechnology



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PODROČJA DEJAVNOSTI

Raziskave v laboratoriju so usmerjene v raziskave bioloških procesov, kot sta prepoznavanje bioloških makromolekul in prenos signalov v celicah in imajo potencialno uporabnost (predvsem biotehnoško, medicinsko, farmaceutsko). Pri tem uporabljamo moderne metode biokemije, molekularne biologije, mikrobiologije in biofizike.

Raziskave s področja medicine se nanašajo na molekularne mehanizme sepse, konformacijskih bolezni in strukture amiloidov in delovanja antimikrobnih učinkovin. Zanimajo nas mehanizmi prepoznavanja in biološke aktivnosti na molekularni ravni, zlasti molekularnih vzorcev, značilnih za patogene mikroorganizme (PAMP), zato uporabljamo instrumentalne metode z visoko ločljivostjo in občutljivostjo, kot sta jedrska magnetna resonanca (NMR) in fluorescenčna spektroskopija. Raziskave vključujejo študij fiziologije mikroorganizmov, ki izločajo encime, organske kisline, antibiotike in druge zdravilne učinkovine kot tudi rekombinantne proteine. Laboratorij vzdržuje mikrobiološko zbirko (MZKI), v kateri hranimo več kot 3000

RESEARCH ACTIVITIES

Activity at the department is oriented towards research of the biochemical processes, particularly molecular recognition and signal transduction, and towards the application of modern biochemical, biotechnological, microbiological, biophysical and molecular biological methods to problems, which have potential industrial application in fields such as medicine, pharmacy or biotechnology.

Research topics with application in medicine are molecular mechanisms of sepsis, conformational diseases and antimicrobial activity of (lipo)peptides. We are interested in the mechanism of recognition of pathogen associated molecular patterns (PAMPs) at the molecular level where we are employing methods with high resolution such as nuclear magnetic resonance and fluorescence spectroscopy. Research interests include study of metabolic regulation in microorganisms, which are able to excrete a number of useful bioproducts, such as enzymes, organic acids, antibiotics and other pharmaceuticals, as well as recombinant proteins. Department hosts the Microbial Culture Collec-

sevov mikroorganizmov, predvsem ekstremofilnih gliv in jo redno dopolnjujemo z novimi izolati.

BIBLIOGRAFIJA

- 7 izvirnih znanstvenih člankov
- 1 strokovni članek
- 1 poljudni članek
- 1 polemika, diskusija, prispevek
- 1 intervju
- 1 priročnik, slovar, leksikon, atlas, zemljevid
- 1 objavljeni znanstveni prispevek na konferenci
- 16 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 3 patentne prijave
- 7 predavanj na tujih univerzah
- 3 prispevki na konferencah brez natisa
- 1 vabljen predavanje na konferenci brez natisa
- 1 elaborat, predštudija, študija
- 2 diplomi
- 1 magisterij

GLAVNI DOSEŽKI V LETU 2006

V letu 2006 smo, skupaj s partnerji v konzorciju, pridobili in začeli uporabljati laserski fluorescenčni konfokalni mikroskop Leica DMI-3000B, ki bo omogočil upodabljanje živih celic, vključno z izraženimi fluorescenčnimi proteini. Ugotovili smo, da katehini iz zelenega čaja, predvsem EGCG, inhibirajo bakterijsko girazo, kar je najbrž podlaga antimikrobnega delovanja zelenega čaja. Ugotovili smo, da se katehini vežejo na enako mesto kot ATP, kjer z njim tekmujejo za vezavo na encim. S pomočjo NMR spektroskopije visoke ločljivosti smo ugotovili vezalno mesto EGCG na N-terminalnem fragmentu giraze B, kar predstavlja osnovo za načrtovanje novih učinkovin z manjšimi stranskimi učinki, saj je zeleni čaj že tisočletja prisoten v človeški prehrani. Rezultate smo objavili v vodilni reviji na področju kemije zdravlil in naleteli na velik odziv v javnosti. Tako so o

tion, with more than 3,000 different strains, with emphasis on extremophiles, which is regularly expanded by new species isolated from their natural environment.

BIBLIOGRAPHY

- 7 Original Scientific Articles
- 1 Professional Article
- 1 Popular Article
- 1 Polemic, Discussion
- 1 Interview
- 1 Manual, Dictionary, Lexicon, Atlas, Map
- 1 Published Scientific Conference Contribution
- 16 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 3 Patent Applications
- 7 Invited Lectures at Foreign Universities
- 3 Unpublished Conference Contributions
- 1 Unpublished Invited Conference Lecture
- 1 Treatise, Preliminary Study, Study
- 2 Undergraduate Theses
- 1 Master's Thesis

MAIN ACHIEVEMENTS IN 2006

In 2006 we and our partners in the consortium acquired a laser fluorescent confocal microscope Leica DMI3000B and set it up in our Laboratory. The microscope will allow us imaging of living cells expressing fluorescent proteins. Among the scientific achievements we can mention the discovery that catechins from green tea, especially EGCG, inhibit the activity of bacterial gyrase, which probably contributes to the antimicrobial activity of green tea. We discovered that catechins bind to the same site as ATP where they compete for the binding to the enzyme. By means of high resolution NMR spectroscopy we have determined the binding site of EGCG at the N-terminal fragment of gyrase B, which may represent the basis for designing antimicrobial drugs with less side effects, since green tea has been used in human nutrition for millennia. We published the

delu poročali na več deset spletnih straneh po vsem svetu, z avtorji dela je bil tudi objavljen intervju v dnevnikih časopisih in na radiu.

Na področju raziskav nevtralizacije bakterijskega endotoksina in antimikrobnih peptidov smo določili prostorske strukture več (lipo)peptidov v okolju membranskih mimetikov. S tem smo ugotovili osnovo za izboljšanje antimikrobne aktivnosti peptidov preko acilacije. Delo je bilo nadaljevanje sicer zaključenega EU projekta ANEPID. Del rezultatov projekta smo prijavi kot patent v Avstriji, nekaj rezultatov smo objavili v članku v reviji *J. Am. Chem. Soc.*, ki je bil sprejet v tisk konec leta 2006.

Velik del raziskav v laboratoriju je potekal na področju imunskega prepoznavanja bakterijskih infekcij. Te raziskave bodo omogočile identifikacijo in razvoj inhibitorjev, ki bi preprečevali pretiran odziv na infekcijo ter na nekatera kronična vnetja, pri katerih sodelujejo receptorji družine Toll. Ugotovili smo, da se spojina bisANS veže na vezalno mesto bakterijskega endotoksina, kar kaže na enostaven strukturni vzorec, ki ga prepozna receptor MD-2. Prav ta protein smo raziskovali kot tarčo za inhibicijo. V sodelovanju z raziskovalci z Univerze v Iowi (ZDA) smo analizirali vpliv mutacij MD-2 na vezavo LPS, kar nam bo omogočilo razumevanje razlik odziva mišjega in človeškega receptorja.

V letu 2006 smo raziskovali mehanizem in diagnostiko prionskih bolezni, predvsem v povezavi z EU projektom TSEUR. Tako smo ugotovili selektivno vezavo kurkumina na prionski protein s spremenjeno konformacijo. Kurkumin namreč preprečuje pretvorbo *in vitro* ter v celičnih linijah, pokazali pa so tudi njegovo učinkovitost na modelu Alzheimerjeve bolezni. S pomočjo spektroskopskih tehnik smo ugotovili jakost vezave ter posredno tudi ultrastrukturo prionskih fibril.

Razvili smo novo metodo za stereospecifično asignacijo resonanc v NMR spektrih na osnovi tridimenzionalne strukture oz. modela in NMR spektrov. Sodelovali smo pri določitvi strukture kompleksa med citokromom c in oksidazo.

S pomočjo novega konfokalnega mikroskopa

results in the leading journal in the field of medicinal chemistry and our results were welcomed by a significant public response. There were reports about this research on numerous web pages, interviews with the authors have been published in daily newspapers and broadcasted by the radio.

In the area of neutralisation of bacterial endotoxin and antimicrobial peptide research we have determined the spatial structures of several (lipo)peptides in the membrane mimetic environment. In such a way we found out the basis for the improvement of antimicrobial activity of peptides through acylation. This research was a continuation of an already finished EU project ANEPID. A patent application has been filled-in in Austria; and additional results were accepted for publication in the *J. Am. Chem. Soc.* at the end of 2006.

A great deal of the research in our Laboratory represented the investigation of the molecular mechanism of immunological recognition of bacterial infections. These investigations will enable identification and development of inhibitors that will prevent exaggerated reaction to the infection and to chronic inflammation involving Toll-like family receptors. We discovered that the compound bisANS binds to the same binding site as bacterial endotoxin, which indicates a simple structural pattern that is recognised by the receptor MD-2. We specifically studied this protein as the target for inhibition. In cooperation with researchers from the University in Iowa (USA) we analysed the effect of mutations of MD-2 on the binding of LPS which, will enable us to understand the differences in the responses between murine and human receptors.

In 2006 we also studied mechanism and diagnostics of prion diseases, mainly in connection with the EU project TSEUR. We found a selective binding of curcumin to a prion protein with a changed conformation. Curcumin prevents transformation *in vitro* as well as in neuroblastoma cell lines, additionally its effectiveness was

smo uspeli upodobiti znotrajcelične vrednosti pH gliv, tako da smo uporabili inovativen genetsko kodirani pH biosenzor, ki temelji na zelenem fluorescirajočem proteinu ter znotraj celični koncentraciji prostih kalcijevih ionov. Senzor za kalcij smo v povezavi z University of Edinburgh analizirali z metodo FLIM-FRET (Förster Resonance Energy Transfer in Fluorescence Lifetime Imaging Microscopy), ki je potrdila možnost uporabe omenjenega sensorja v glivah. Z rekombinatnim sensorjem za pH smo določili znotraj celično pH vrednost pri glivah in potrdili, da je uravnavanje znotrajcelične vrednosti pH povezano z uravnavanjem znotrajcelične koncentracije kalcija, saj pri glivah z okvarjenimi kalcijevimi črpalkami pride do dviga znotrajcelične vrednosti pH. Pripravili smo celične linije HEK, ki vsebujejo rekombinantni senzor aequorin, ki omogoča spremljanje sprememb koncentracije prostih kalcijevih ionov. Spremembe v koncentraciji kalcija spremljamo ob aktivaciji sistemskega vnetnega odgovora. V preteklem letu smo v ugledni ameriški reviji

shown on a model of Alzheimer disease. By means of spectroscopic techniques we determined the strength of binding and indirectly also the ultrastructure of prion fibrils.

We developed a new method for stereospecific assignment of resonances in the NMR spectra on the basis of a three-dimensional structure or a structural model. We participated in the structural determination of a complex between the cytochrome c and oxidase.

By means of the new confocal microscope we succeeded to determine the intracellular pH values by the use of an innovative, genetically coded pH biosensor, which relies on the green fluorescent protein and intracellular concentration of free calcium ions. In collaboration with the colleagues from the University of Edinburgh the sensor for calcium was analysed by a method FLIM-FRET (Förster Resonance Energy Transfer in Fluorescence Lifetime Imaging Microscopy), which confirmed the possible use of the mentioned sensor in fungi. With the recombinant sensor for the pH we determined the intracellular pH value in fungi and confirmed



SLIKA 1:
Delo na laserskem konfokalnem fluorescenčnem mikroskopu Leica DMI3000B

FIGURE 1:
Working on Lasers confocal microscope Leica DMI3000B

objavili še en članek, ki opisuje spontano post-translacijsko modifikacijo ključnega regulatornega encima primarnega metabolizma 6-fosfofruktokinaze (PFK1). Dokazali smo, da ima modifikacija proteinske molekule za posledico spremembo encimske kinetike, tako da encim ni več občutljiv na inhibicijo povratne zveze, medtem ko nekateri celični aktivatorji omogočajo hitrejšo bio-katalizo. Sprememba encima in posledično nastanek aktivnega krajšega fragmenta povzroči neoviran pretok metabolitov preko glikolize, dvig koncentracije intermediatov centralnega dela metabolizma in ojačane anabolne reakcije, vključno s povečano sintezo specifičnih biotehnoloških produktov.

Na povabilo urednika tuje biotehnološke revije je dr. Legiša v sodelovanju s tujim avtorjem napisal pregledni članek o metabolnih spremembah med zgodnjim razvojem pri glivi *A. niger*, ki pripeljejo do prekomernega izločanja organske kisline. V članku je predstavljen specifičen pogled avtorjev na spremembe v metabolizmu, kjer igra osrednjo vlogo predvsem post translacijska modifikacija PFK1. Da gre pri tem delu za rekapitulacijo večletnih raziskav prvega avtorja (dr. Legiše), priča tudi dejstvo, da se od 49 referenc, kolikor jih vsebuje dokument, kar 9 nanaša na avtorjeve članke.

S namenom, da bi se izognili zapleteni post translacijski modifikaciji PFK1, smo pripravili modificiran gen *pfkA*, ki nosi zapis za aktiven krajši fragment PFK1. Z vnosom gena v nekaj komercialno uporabnih mikroorganizmov smo v primerjavi s starševskimi sevi pri transformantah opazili pospešeno rast oziroma povečano hitrost sinteze določenih bio produktov, kot so organske kisline in ekstracelularni encimi. Uporabo modificiranega gena za dvig produktivnosti in dobitkov pri pridobivanju različnih biotehnoloških produktov smo patentno zaščitili. Z namenom, da bi rezultate raziskovalnega dela prenesli v prakso, smo nekaterim uporabnikom ponudili prenos intelektualne lastnine, ki je zaobjeta v zgoraj opisanem patentu. Trenutno potekajo pogovori s tujim biotehnološkim podjetjem o odprodaji licenčnih pravic.

that regulation of the intracellular pH value was connected to regulation of intracellular calcium concentration since in fungi with damaged calcium pumps the intracellular pH increased. We prepared HEK cell lines including a recombinant sensor aequorin, which enables tracing the concentration changes of the free calcium ions.

In a distinguished scientific journal we published another publication, which describes the spontaneous posttranslational modification of 6-phosphofructokinase (PFK1), the key regulation enzyme of the primary metabolism. We proved that a modification of the protein molecule resulted in a change of the enzyme kinetics in such a way that the enzyme was no longer sensitive to feedback inhibition by citrate, while some cell activators enabled faster biocatalysis. The change of the enzyme and a consequent formation of the active shorter fragment led to an unimpeded flow of metabolites through glycolysis, increase of concentration of the intermediates of the central part of metabolism and the strengthening of the anabolic reactions including the increased synthesis of specific biotechnological products. At the invitation of the editor of a distinguished biotechnological journal Dr. Legiša in cooperation with a foreign author wrote a review article on the metabolic changes during the initial development of the fungus *A. niger*, which led to excessive excretion of an organic acid. A specific authors' view of the metabolic changes is presented where the posttranslational modification of PFK1 plays the central role. With the aim to avoid the complex posttranslational modification of PFK1 we prepared a modified *pfkA* gene encoding for the active shorter fragment of the PFK1. By inserting the gene into some commercially useful microorganisms accelerated growth and/or synthesis of certain products has been noticed in transformants, such as accumulation of organic acids and excretion of extracellular enzymes in respect to the parent strains. The use of the modified gene for increased productivity and yields in the production of different bio-

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Lek d.d., Ljubljana: raziskave na področju biotehnologije ter razvoja novih zdravil
- BIA Separations d.o.o, Ljubljana, dva skupna projekta
- KIMI d.o.o., Trzin

MEDNARODNO SODELOVANJE

V mednarodnih projektih:

- dva evropska projekta v okviru 6. okvirnega programa: Eurofungbase in TSEUR
- bilateralno sodelovanje s Hrvaško, ZDA, Indijo, Francijo in Argentino
- COST projekt D25: »Applied biocatalysis: Stereoslective and environmentally-friendly reactions catalysed by enzymes«

Pogodbe s podjetji v tujini:

- Colgate Palmolive, ZDA
- DSM Food Specialists, Nizozemska
- LVMH, Christian Dior Parfums, Francija
- IEP GmbH, Germany

Neformalno sodelovanje z drugimi znanstvenimi ustanovami po svetu:

- University of Sussex, UK
- University of Strathclyde, Glasgow, Škotska
- The University of Edinburgh, Edinburgh, Škotska
- Technische Universität Graz, Avstrija
- Universidad de Navarra, Pamplona, Španija
- Indian Institute of Science, Bangalore, Indija

POMEMBNI INŠTRUMENTI IN OPREMA

- Pretočni citometer s sorterjem EPICS® ALTRA™, Beckman Coulter,
- laserski konfokalni fluorescenčni mikroskop Leica DMI3000B,
- CD spektrometer Chirascan, Applied Photo-physics,
- UV/VIS spektrometer, Perkin Elmer Lambda 25,

technological products was protected by a patent. With the aim to transfer the research results into practice we offered the intellectual property rights to some beneficiaries. At the moment, we are having discussions with a biotechnological company for licensing out the IP rights.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Lek, d.d., Ljubljana, Slovenia: research of fungal metabolism and molecular biology of *Streptomyces*
- BIA Separations d.o.o, Ljubljana, Slovenia: two joint projects
- KIMI d.o.o., Trzin, Slovenia

INTERNATIONAL COLLABORATION

International projects:

- Two projects within the 6th Framework Program: Eurofungbase and TSEUR
- Bilateral projects with USA, France, India, Croatia and Argentina
- COST project D25: "Applied biocatalysis: Stereoslective and environmentally-friendly reactions catalysed by enzymes"

Contracts with companies abroad:

- Colgate Palmolive, USA
- DSM Food Specialists, The Netherlands
- LVMH, Christian Dior Parfums, France
- IEP GmbH, Germany

Informal collaboration with other research institutions:

- University of Sussex, UK
- University of Strathclyde, Glasgow, UK
- The University of Edinburgh, Edinburgh, UK
- Technische Universität Graz, Austria
- Universidad de Navarra, Pamplona, Spain
- Indian institute of Science, Bangalore, India

- fluorescenčni luminometer, Perkin Elmer LS-55,
- luminometer/fluorimeter za mikrotitrnske plošče z injektorjem, Mitras,
- grafična postaja Silicon Graphics Fuel s programsko opremo za NMR, molekularno modeliranje in SAR,
- bioreaktorji: Infors,
- FIA (flow injection analyser),
- HPLC in drugi kromatografski instrumenti,
- sistem za 2D elektroforezo s programsko opremo (Melanie),
- laboratorij za delo z mikroorganizmi,
- laboratorij za delo s celičnimi kulturami.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Pet sodelavcev L12 je habilitiranih za sodelovanje pri do- in podiplomskem študiju Univerze v Ljubljani.
- Opravljeni sta bili dve diplomski deli in eno magistrsko delo.
- Gostovanje podiplomskega študenta Gorana Mikluševića iz Hrvaške in podiplomske študentke Kirsten Altenbach iz Velike Britanije.

ODMEVEN DOSEŽEK V MEDIJIH

Raziskovalci Laboratorija za biotehnologijo so v sodelovanju z doc. Dolinarjem s Fakultete za kemijo in kemijsko tehnologijo, Univerze v Ljubljani organizirali sodelovanje študentske ekipe na tekmovanju iGEM (international Genetically Engineered Machines). V okviru tega sodelovanja študentske ekipe med počitnicami v nekaj mesecih pripravijo raziskovalni projekt s področja sintezne biologije. Na izboru članov ekipe smo izbrali sedem študentov mikrobiologije in biokemije. Pri izvedbi projekta so kot mentorji sodelovali štiri raziskovalci Laboratorija za biotehnologijo Kemijskega inštituta, dejansko pa je pri delu pomagalo veliko število članov laboratorija. Projekt je bil

MAJOR EQUIPMENT

- The EPICS® ALTRA™ Flow Cytometer, Beckman Coulter
- Lasers confocal microscope Leica DMI3000B
- CD spectrometer Chirascan, Applied Photophysics
- UV/VIS spectrometer, Perkin Elmer Lambda 25
- Fluorescence luminometer PerkinElmer LS-55
- Microplate luminometer/fluorimeter with injectors
- Graphical workstation Silicon Graphics Fuel with software for NMR, molecular modeling and SAR analysis
- Bioreactors: Infors
- FIA (Flow Injection Analyser)
- HPLCs
- System for 2D gel electrophoresis with software for data evaluation (Melanie)
- Laboratories for microbiology and cell culture

EDUCATION AND IMPORTANT VISITS

- Five members of the Laboratory of Biotechnology participate as lecturers or demonstrators at the under- and postgraduate level at the University of Ljubljana, Slovenia.
- Two BSc projects and one MSc project performed at the department have been defended in 2006.
- Research visits of PhD students Goran Miklušević from Croatia and Kirsten Altenbach from United Kingdom.

ACHIEVEMENT NOTED IN THE MEDIA

Researchers of the Laboratory of Biotechnology in cooperation with Asst. Prof. Marko Dolinar from the Faculty of Chemistry and Chemical Technology, University of Ljubljana, organized the participation of a student team from Slovenia at the international competition iGEM (international Genetically Engineered Machines) in the frame of which student teams worked

usmerjen v spreminjanje lastnosti odziva celic na bakterijsko infekcijo. Projekt je bil s področja raziskav L12, to je celične signalizacije bakterijske infekcije. V projektu so v kaskado celične signalizacije vgradili povratno zanko, preko katere so inhibirali pretiran celični odziv s pomočjo dominantno negativne mutante ključnega adapterja v signalizaciji MyD88 (predstavitev projekta se nahaja na spletni strani http://parts2.mit.edu/wiki/index.php/Ljubljana%2C_Slovenia_2006).

Tekmovanje na univerzi MIT v Cambridge-u v ZDA je potekalo v začetku novembra 2006. Med sodelujočimi ekipami so bile skupine z najuglednejših svetovnih univerz in inštitutov, kot so: Berkeley, Princeton, Caltech, Harvard, Massachusetts Institute of Technology (MIT), UCSF, Imperial College London, Cambridge in ETH Zürich. Med 34 univerzitetnimi ekipami na iGEM 2006 jih je bilo 25 s seznama najboljših 100 univerz na svetu (kitajski seznam Top500), od teh jih je bilo 13 celo izmed prvih 50. Slovenska ekipa je nastopila v konkurenci z ekipami štirih izmed najboljših pet univerz na svetu (Harvard, Cambridge, Berkeley, MIT; manjkal je samo

on a research project in the field of synthetic biology during their holidays. Out of many candidates seven students of microbiology or biochemistry were finally selected.

Four researchers from the Laboratory of Biotechnology at NIC were involved as mentors, but in fact many members of the lab helped in the project. The focus of the project was to modify the characteristics of cellular response to bacterial infection. This fits within the research topic of our lab in the area of cell signalling to bacterial infection. Within the project a feedback loop with a dominant negative inhibitor under the control of NF-KB promotor was incorporated into the cell signalling cascade and through this loop an excessive cell response was inhibited by means of a dominant negative mutant of the key adapter in signalisation MyD88 (presentation of the project is available at:

http://parts2.mit.edu/wiki/index.php/Ljubljana%2C_Slovenia_2006).

The competition took place at MIT in Cambridge, USA at the beginning of November 2006. Among the participating teams there



SLIKA 2:

Zmagovalna slovenska ekipa na tekmovanju iGEM na MIT, v kateri so sodelovali mentorji iz Laboratorija za biotehnologijo Kemijskega inštituta (sredina – zelene majice) skupaj z ekipama finalistov Imperial college (levo) in Princetona (desno).

FIGURE 2:

Victorious Slovenian team at the iGEM competition where the researchers from the Laboratory of Biotechnology at NIC were involved as mentors (centre – green T-shirts) together with the other two finalist teams from the Imperial College (left) and Princeton (right).

Stanford, ki je na tretjem mestu). V konkurenci ekip najboljših svetovnih univerz se je naša ekipa najprej uvrstila v finale, skupaj z ekipama univerz Princeton ter Imperial College. Vsi finalisti so še enkrat predstavili svoje projekte vsem sodelujočim s 35 univerz s celega sveta. Po odločitvi sodnikov je ljubljanska ekipa zasedla prvo mesto. Poleg najbolj cenjene skupne prve nagrade (Grand Prize) je ekipa osvojila še dve drugi in eno tretje mesto v posameznih kategorijah. Projekt je vključeval tudi računalniško simulacijo spremenjenega delovanja celičnih procesov, saj gre za medsebojno delovanje velikega števila celičnih sestavin ter povratnih zank. Projekt, ki si ga je po temeljitih razmisleku ekipa izbrala, je glede na dosedanje teme na tekmovanjih iGEM dokaj zahteven, zato so z delom na projektu, katerega rezultate so predstavili na novembrskem srečanju tekmovalnih ekip, začeli že maja. Doslej so ekipe namreč uporabljale preprostejše organizme (bakterije in kvasovke), dela z gojenimi sesalskimi celicami pa se doslej ni lotila še nobena ekipa.

Rezultati tekmovanja so bili deležni izjemnega odziva predvsem v tujini, o uspehu je poročala revija Nature, največje svetovne agencije s področja znanosti, v Sloveniji pa v člankih v dnevnikih, v radijskih ter televizijskih intervjujih. Predstavitev projekta na tekmovanju je dostopna na svetovnem spletu v obliki videoposnetka: <http://www.igem2006.com/presentations.htm>.

were groups from the most prominent universities and institutes worldwide, such as Berkeley, Princeton, Caltech, Harvard, MIT, UCSF, Imperial College London, Cambridge, ETH In the competition our team first got into the final, together with the teams from the universities Princeton and Imperial College. All the finalists had to present their projects once again to all of the participants. According to the decision of the judges the Slovenian team won the first place. In addition to the most esteemed Grand Prize our team also won two second and one third place in separate categories. The project included also a computer simulation cell signalling. In comparison to the previous projects at iGEM competitions our project was relatively demanding. In previous years the teams worked with simple unicellular organisms (bacteria and yeasts), while none worked with cultured mammalian cells.

The results of the competition met with a significant response, especially abroad. Success was reported in the journal Nature, by world news agencies in the field of science, in Slovenia there were articles in daily newspapers, and interviews on radio and TV. The project presentation at the meeting is available on the Internet in a form of the video at the page: <http://www.igem2006.com/presentations.htm>

L13

Laboratorij za katalizo in
reakcijsko inženirstvo

Laboratory for Catalysis and
Chemical Reaction Engineering



VODJA / HEAD

Akademik prof. dr. Janez Levec

RAZISKOVALCI / RESEARCHERS

Dr. Jurkica Batista
Dr. Gorazd Berčič
Dr. Stanko Hočevar
Dr. Henrik Kušar
Dr. Albin Pintar

**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Matej Komel
Luka Zevnik



PODROČJA DEJAVNOSTI

Študij kemijskih pretvorb različnih izhodnih spojin v zelene produkte v homogenih in heterogenih kataliziranih ali nekataliziranih sistemih. Teoretična določitev termodinamskih možnosti za potek pretvorb in eksperimentalna določitev kinetičnih parametrov poteka teh pretvorb. Ker v praksi večina fizikalnih in kemijskih pretvorb poteka v večfaznih sistemih, je velik del raziskav namenjenih študiju interakcij kemijske kinetike s transportnimi pojavi. Raziskave potekajo s poudarkom na:

- oksidaciji organskih polutantov v membranskih reaktorjih,
- optimizaciji hidrodinamskih pogojev obratovanja eno- in več cevnih membranskih kontaktorjev,
- interpretaciji eksperimentalnih meritev na podlagi matematičnega modeliranja in optimizacije parametrov,
- razvoju Pd-Cu bimetalnih in Pd monometalnih katalizatorjev, uporabljenih v integriranem procesu za denitrifikacijo podtalnice,

RESEARCH ACTIVITIES

Study of the chemical transformation of reactants to desirable products in homogeneous and heterogeneous catalytic or non-catalytic systems. Theoretical determination of thermodynamic possibility for certain transformation and experimental determination of kinetic parameters for these transformations. In practice most physical and chemical transformations occur in the multiphase systems, therefore research efforts are focused on the study of the interaction between intrinsic kinetics and transport phenomena. The emphasis of the research is put on:

- catalytic wet oxidation of organics dissolved in wastewater carried out in membrane reactors;
- optimization of process hydrodynamic conditions in single- and multi-channel membrane contactors;
- interpretation of experimental data through mathematical modelling and optimization of parameters;
- development of Pd-Cu bimetallic and Pd

- kinetičnim in mehanističnim študijam heterogeno kataliziranih reakcij z *in-situ* FTIR/ATR metodo,
 - študiju kinetike in mehanizmov kataliziranih reakcij v procesih proizvodnje in čiščenja vodika ter načrtovanju kompaktnega procesorja za proizvodnjo vodika iz primarnih goriv (fosilnih in obnovljivih) za PEM gorivne celice,
 - sintezi ter strukturalni in elektrokemični karakterizaciji novih anodnih katalizatorjev, odpornih na CO, za uporabo v PEM gorivnih celicah,
 - sintezi ter strukturalni elektrokemični karakterizaciji nanokompozitnih protonsko prevodnih polimernih membran za PEM gorivne celice.
- monometallic catalysts for integrated process of underground drinking water denitrification;
 - kinetic and mechanistic studies of heterogeneously catalyzed reactions with *in situ* FTIR/ATR method;
 - study of kinetics and mechanisms of catalyzed reactions in the hydrogen production and cleaning processes from primary fuel sources (fossil and renewable) for PEM fuel cells;
 - synthesis, structural and electrochemical characterization of new CO-tolerant anode catalysts for PEM fuel cells;
 - synthesis, structural and electrochemical characterization of proton conducting nanocomposite polymer membrane for PEM fuel cells.

BIBLIOGRAFIJA

- 6 izvirnih znanstvenih člankov
- 1 samostojni znanstveni sestavek v monografiji
- 2 objavljena znanstvena prispevka na konferencah
- 5 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 patentna prijava
- 1 predavanje na tuji univerzi
- 2 prispevka na konferencah brez natisa
- 2 elaborata, predštudiji, študiji
- 1 magisterij
- 2 uredništvu revij

DOSEŽKI V LETU 2006

- Na primeru modelne reakcije (oksidacije vodne raztopine mravljične kisline na Pt katalizatorju, nanešenem na keramični cevni membrani) smo za široko območje obratovnih pogojev razvili matematični model za napoved koncentracijskih profilov reaktantov in debelino reakcijske cone v katalitskem trifaznem membranskem reaktorju. COBISS.SI-ID 3428122
- Z uporabo dveh ločenih katalitskih reaktorjev, napolnjenih s Pd-Cu oziroma Pd katalizatorjem, smo modificirali procesno shemo

BIBLIOGRAPHY

- 6 Original Scientific Articles
- 1 Independent Scientific Component Part in a Monograph
- 2 Published Scientific Conference Contributions
- 5 Published Scientific Conference Contribution Abstracts
- 1 Patent Application
- 1 Invited Lectures at Foreign University
- 2 Unpublished Conference Contributions
- 2 Treatises, Preliminary Studies, Studies
- 1 Master's Thesis
- 2 Journal Editorships

RESULTS IN 2006

- On the basis of catalytic wet-air oxidation of aqueous solutions of formic acid investigated as a model reaction over Pt-doped ceramic membranes in a wide range of operating conditions, a comprehensive mathematical model for the prediction of both concentration profiles of reactants and the thickness of reaction zone in the catalytic membrane reactor was developed. COBISS.SI-ID 3428122

- integriranega procesa za odstranjevanje presežnih množin nitratnega iona iz pitne vode, s čimer se je drastično zmanjšala produkcija amonijevega iona kot stranskega produkta reakcije. COBISS.SI-ID 3408410
- Določili smo kinetiko reakcije vodnega plina (water gas shift reaction, WGSR) na različno sintetiziranih nanostrukturnih $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-y}$ katalizatorjih v stacionarnih pogojih z različnimi sintetičnimi izhodnimi mešanicami plinov, ki simulirajo sestavo plinov po reformingu primarnega goriva (metana oziroma premoga) in pokazali, kako močno vplivajo pogoji sinteze katalizatorjev na njihovo strukturo in morfologijo ter posledično na njihovo aktivnost in selektivnost v dani reakciji. COBISS.SI-ID 3569946.
 - Objavili smo samostojno poglavje v učbeniku
 - A modified process scheme of the integrated ion-exchange/catalytic denitrification process for the removal of excessive quantities of nitrates from drinking water was proposed by introducing separate reactor units filled with Pd-Cu bimetallic and Pd monometallic catalysts, respectively, which drastically reduces the production of ammonium ions as a by-product. COBISS.SI-ID 3408410
 - Kinetic model of water gas shift reaction (WGSR) over a nanostructured $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-y}$ catalysts prepared with different methods was determined based on measurements under stationary reaction conditions with simulated reformer outlet gas mixtures (obtained from methane or coal). It was confirmed that conditions for catalysts preparation decisively influence on the structure and



SLIKA:
Računalniško vodeni kontinuirni reaktorski sistem »Microactivity Reference« za študij dvo- in trifaznih katalitskih reakcij pri temperaturah do 750 stopinj Celzija in tlakih do 100 bar (PID Eng&Tech, Španija)

FIGURE:
Computerized continuous-flow reactor system »Microactivity Reference« for studies of two- and three-phase catalytic reactions at temperatures up to 750 degrees C and pressures up to 100 bar (PID Eng&Tech, Spain)

(S. Hočevar) za podiplomski študij katalize pod naslovom »Surface and Nanomolecular Catalysis« (R. Richards, ur.), CRC Taylor & Francis, Boca Raton, FL, USA, 2006. COBISS.SI-ID 3486490

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Za Ministrstvo za obrambo RS (MORS) smo opravili dve izvedljivostni študiji s področja vodikovih tehnologij in gorivnih celic (štev. pog. 4300-958/2006-1, nosilec: dr. Gorazd Berčič; štev. pog. 4300-957/2006-1, nosilec: dr. Stanko Hočevar);
- za slovensko farmacevtsko družbo smo izvedli evaluacije in optimizacije različnih industrijskih procesov (npr. industrijskega procesa katalitske hidrogenacije; nosilec: prof. dr. Janez Levec).

MEDNARODNO SODELOVANJE

- »Polymer Electrolytes and Non Noble Metal Electrocatalysts for High Temperature PEM Fuel Cells« v okviru EU 6 FP programa »Integrating and Strengthening of European Research Area« STREP projekt NMP3-CT-2006-033228 (Akronim: APOLLON-B). Projekt traja od 01. 10. 2006 do 01. 10. 2009, koordinator projekta na KI je dr. Stanko Hočevar.

POMEMBNI INŠTRUMENTI IN OPREMA

- Računalniško voden tekočinski kromatograf (HP),
- več plinskih kromatografov s TCD in FID detektorjem (HP),
- analizatorja vsebnosti ogljika v tekočih in trdnih vzorcih (Tekmar/Dohrmann),
- več mešalnih šaržnih, kapalnih in cevnih reaktorjev s strnjnim slojem opremljenih s sistemi za nadzor in zajemanje podatkov,
- 600 W sistem za testiranje gorivnih celic z računalniškim vodenjem (HP VEE OneLab),
- LabMax-ReactIR 1000 mešalni šaržni reaktor s sistemom za IR analizo reakcije v realnem času (Mettler Toledo),

morphology of the catalysts and consequently on their activity and selectivity in given reaction. COBISS.SI-ID 3569946

- A chapter was published (S. Hočevar) in the book for graduate course under the title »Surface and Nanomolecular Catalysis« (R. Richards, Ed.), CRC Taylor & Francis, Boca Raton, FL, USA, 2006. COBISS.SI-ID 3486490

COLLABORATION WITH COMPANIES

- Two feasibility studies were performed for MoD RS (MORS) in the field of hydrogen technology and fuel cells (CT 4300-958/2006-1, PI dr. Gorazd Berčič; CT 4300-957/2006-1, PI dr. Stanko Hočevar).
- For a Slovenian pharmaceutical company the industrial scale hydrogenation process was optimised (PI prof. dr. Janez Levec).

INTERNATIONAL COLLABORATION

- »Polymer Electrolytes and Non Noble Metal Electrocatalysts for High Temperature PEM Fuel Cells« STREP Project in EU 6 FP »Integrating and strengthening of European Research Area«, NMP3-CT-2006-033228 (Acronym: APOLLON-B). Project lasts from 01.10.2006 to 01.10.2009; Project coordinator within NIC is Dr. Stanko Hočevar.

IMPORTANT INSTRUMENTS AND EQUIPMENT

- HPLC + ChemStation (HP)
- several GCs with TCD and FID detector (HP)
- TOC analyzers in liquid and solid samples (Tekmar/Dohrmann)
- several batch CST, trickle-bed and fixed-bed laboratory reactors with data acquisition and control units
- 600 W fuel cell test station with HP VEE OneLab software-based data acquisition and control unit
- LabMax-ReactIR 1000 reactor and real-time reaction analysis system (Mettler Toledo)

- avtomatizirani sistem za karakterizacijo heterogenih katalizatorjev (Micromeritics, model Autochem II 2920),
- masni spektrometer (Pfeiffer Vacuum, model Thermostar),
- računalniško vodeni, kontinuirni reaktorski sistem »Microactivity Reference« za študij dvo- in trifaznih katalitskih reakcij pri temperaturah do 750 stopinj Celzija in tlakih do 100 bar (PID Eng&Tech, Španija).
- Automated system for heterogeneous catalysts characterization (Micromeritics, model Autochem II 2920)
- Mass spectrometer (Pfeiffer Vacuum, model Thermostar)
- Computerized continuous-flow reactor system »Microactivity Reference« for studies of two- and three-phase catalytic reactions at temperatures up to 750 degrees C and pressures up to 100 bar (PID Eng&Tech, Spain)

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

V letu 2006 je bilo zaključeno eno magistrsko delo (M. Komel: *Numerično določevanje parametrov prenosa toplote v strnjenih slojih*, magistrsko delo, Ljubljana. [M. Komel], 2006. XVII, 128 f., ilustr. [COBISS.SI-ID 27747077], mentor prof. dr. Janez Levec).

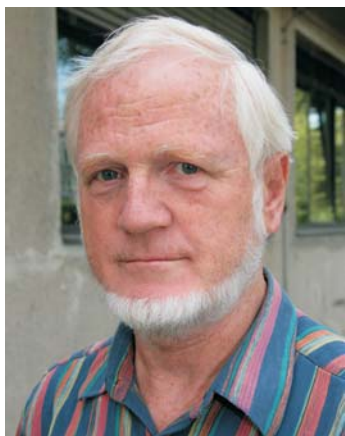
EDUCATION AND IMPORTANT VISITS

One master degree thesis (M. Komel, "Numerical determination of heat transfer parameters in packed beds": M.Sc. Thesis, Supervisor: Professor Janez Levec [COBISS.SI-ID 27747077]) was concluded in 2006.

L14

Laboratorij za procesno inženirstvo

Laboratory for Chemical Process Engineering



VODJA / HEAD
Prof. dr. Viktor Grilc

RAZISKOVALCI / RESEARCHERS

Dr. Ljudmila Fele Žilnik
Mag. Muharem Husić (tudi vodja službe za
zdravje in varnost pri delu KI / also Officer for
occupational safety and health)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Špela Božič
Bojan Robič

PRIPRAVNIKI / TRAINEES

Alma Jazbinšek
mag. Andrej Šonc (do / untill 30. 6. 2006)



PODROČJA DEJAVNOSTI

Razvoj procesov

- Raziskave in razvoj tehnično pomembnih proizvodnih procesov, sodobnih separacijskih tehnik, postopkov za varstvo okolja v kemijski in procesni industriji, trajnostnega industrijskega razvoja; modeliranje in optimiranje delovanja posameznih procesnih elementov in naprav; odpravljanje ozkih grl procesov; izdelava tehnoloških podlag za nove ali inovirane procese; povečevanje novih proizvodnih postopkov iz laboratorijskega v pilotno in polindustrijsko merilo, izvajanje pilotnih poskusov, materialno-energetsko bilanciranje in modeliranje procesov.
- Merjenje izbranih fizikalno-kemijskih lastnosti čistih snovi, mešanic in materialov ter modeliranje termodinamskih ravnotežij večfaznih in večkomponentnih sistemov v širšem obsegu termodinamskih pogojev (tekoče-tekoče, tekoče-parno, tekoče-trdno) za potrebe načrtovanja teh operacij in naprav.

Čiste tehnologije

- Razvoj in integracija preventivnih ukrepov varstva okolja v industrijske procese; uvajanje

RESEARCH ACTIVITIES

Process research and development

- research and development of new industrial products and processes, development of scale-up methods for chemical processes, industrial environmental protection, process simulation and optimization
- measurement of thermodynamic properties (e.g. L-V, L-L and L-S equilibria) of various industrially important multicomponent mixtures in broad range of thermodynamic conditions and their modelling by means of advanced statistical methods
- integration of pollution prevention and environmental protection measures in new or existing industrial/infrastructural processes, development of reclamation processes for recyclable components from process waste streams
- development and implementation of methods and procedures for identification, classification and characterization of hazardous wastes; research and development of pre-treatment processes for difficult effluents and

principov *čistejše proizvodnje* v industrijsko prakso; izdelava ocen skladnosti proizvodnih procesov z *BAT* tehnologijami po direktivi *IPPC*.

- Preprečevanje onesnaževanja okolja; razvoj postopkov za regeneracijo uporabnih komponent iz odpadnih tokov; zapiranje tehnoloških krogov in uvajanje regeneracijskih/reciklažnih postopkov; identifikacija, karakterizacija in klasifikacija odpadkov ter razvoj postopkov obdelave in končnega ravnanja z neogibnimi industrijskimi in drugimi odpadki.

Ekspertize in servisna dejavnost

- Izdelava in revizija poročil o vplivih proizvodnih in drugih procesov na okolje (pooblastilo Ministrstva za okolje in prostor Republike Slovenije);
- izdelava načrtov za gospodarjenje z odpadki in ocen odpadkov (pooblastilo Ministrstva za okolje in prostor Republike Slovenije);
- regeneracija posebno čistih laboratorijskih in procesnih topil (dovoljenje Ministrstva za okolje in prostor Republike Slovenije);
- laboratorijska / pilotna proizvodnja specialnih kemičnih izdelkov;
- ocene in revizije razvojnih, predinvesticijskih in ekoloških projektov.

BIBLIOGRAFIJA

- 3 izvorni znanstveni članki
- 1 strokovni članek
- 1 drugi članek in sestavek
- 2 objavljena strokovna prispevka na konferencah (vabljeni predavanja)
- 4 objavljeni znanstveni prispevki na konferencah
- 2 objavljena strokovna prispevka na konferencah
- 2 objavljena povzetka znanstvenih prispevkov na konferencah
- 2 končni poročili o rezultatih raziskav
- 4 elaborati, predštudije, študije
- 5 izvedenskih mnenj, arbitražnih odločb

hazardous wastes in order to minimize their quantity or hazardness

- national inventories and balances of critical environmental contaminants, wastes and emissions; life cycle assessment, risk assessment; identification and modelling of transport routes of selected contaminants in the environment, elaboration of environmental action programmes.

Clean Technologies

- research, development and implementation of cleaner production principles, pollution prevention and waste minimization measures in the existing and new industrial processes
- assessment of large industrial and environmental protection plants with respect to BAT-requirements, according to IPPC directive and BREF documents.

Expertise and service

- environmental impact assessment studies and reports (upon authorisation)
- waste management plans and waste assessment reports (upon authorisation)
- ISO 14000 and EMAS audits, environmental impact assessments and revisions (upon authorisation)
- Small scale production of specialty chemicals, reclamation of laboratory solvents from waste mixtures, neutralization of hazardous laboratory chemicals.

BIBLIOGRAPHY

- 3 Original Scientific Articles
- 1 Professional Article
- 1 Other Article or Component Part
- 2 Published Professional Conference Contributions (Invited Lectures)
- 4 Published Scientific Conference Contributions
- 2 Published Professional Conference Contributions
- 2 Published Scientific Conference Contribution Abstracts
- 2 Final Research Reports

- 1 diploma
- 1 magisterij
- 2 uredništvi revij

GLAVNI DOSEŽKI V LETU 2006

- Podpis pogodbe in pričetek izvajanja integriranega projekta Evropske unije BIOCOUP v okviru FP6-2004-Energy 3 z naslovom: »Co-processing of upgraded bio-liquids in standard refinery units« (sprejet v financiranje od leta 2006 dalje).
- Pogodba o sodelovanju s firmo Bayer Technology Services Leverkusen, Nemčija, na področju visokotlačnih tehnologij za določanje termofizikalnih lastnosti materialov; v letu 2006 gradnja visokotlačne celice za merjenje faznih ravnotežij. Sodelovanje z Univerzo Erlangen, Nemčija, na področju tvorbe mikrodelcev v farmacevtske namene z uporabo SCF-GAS tehnike.
- Dogradnja državnega informacijskega sistema za področje odpadkov in izdelava nacionalnih bilanc in časovnih trendov nastajanja komunalnih, gradbenih, nevarnih in nevarnih odpadkov, po dejavnostih, povzročiteljih, vrstah odpadkov in načinih ravnanja.
- Sodelovanje pri izdelavi katastra nelegalnih odlagališč odpadkov in predloga sanacije vodozbirnih območij okoli Ljubljane. Izdelava ocene onesnaženosti zemljine s področja stare cinkarne v Celju zaradi sanacije.
- Sodelovanje pri izdelavi tehnoloških podlag za načrtovanje in gradnjo industrijskega postopka čiščenja tehnične fosforne kisline do živilske kvalitete v TKI Hrastnik; sodelovanje pri razvoju tehnološkega postopka priprave natrijevega perkarbonata v Belinki Ljubljana.
- Izvajanje programa razvoja čistih tehnologij za različne kemične proizvode v okviru centra odličnosti Ekološke tehnologije (nosilec Institut Jožef Stefan, Ljubljana), npr. predelava tehnične fosforne kisline v čisto kislino oz. njene soli z uporabo nove generacije ekstraktantov.

- 4 Treatises, Preliminary Studies, Studies
- 5 Expertises, Arbitration Decisions
- 1 Undergraduate Thesis
- 1 Master's Thesis
- 2 Journal Editorships

RESULTS IN 2006

- Start of the integrated EU FP6 project »BIOCOUP« named »Energy 3: Co-processing of upgraded bio-liquids in standard refinery units«. The laboratory is engaged in identification of optimal recovery and fractionation strategies and technologies for the production of discrete target compounds from the bio-liquids and development of technically and economically feasible isolation and fractionation technologies for target oxygenate compounds.
- Construction of high pressure view-cell for determination of thermophysical properties of materials and design of related synthesis and separations (in cooperation with Bayer Technology Services, Leverkusen, Germany). Cooperation with University of Erlangen, Germany.
- Participation in the design of industrial solvent extraction plant for production of pure phosphoric acid from wet P.A. (TKI Hrastnik Chemical Industry, Slovenia); participation in the research of industrial process for sodium percarbonate (Belinka Chemical factory, Ljubljana, Slovenia).
- Upgrade and update of the national information system on waste generation: data collection system for municipal, industrial, construction/demolition and hazardous wastes, generated during the year 2004 in relevant sectors and waste types according to NACE and EWC classification; trends are shown for the time period since 1999.
- Participation in the inventory and assessment of illegal waste sites around the Ljubljana City and preparation of a related reclamation project.
- Analysis and assessment of the contaminated industrial site of old zincworks at Celje.

- Pridobitev pooblastila Ministrstva za obrambo za certificiranje izdelovalcev filtrov za kolektivno zaščito.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- TKI Hrastnik d.d., Hrastnik
- Belinka – Perkemija d.o.o., Ljubljana
- Cinkarna Celje d.d., Celje
- JP Snaga, Ljubljana in JP Vodovod-kanalizacija, Ljubljana
- Agencija RS za okolje, Ministrstvo za okolje in prostor, Ljubljana
- Regionalna razvojna agencija Celje, d.o.o., Celje idr.

MEDNARODNO SODELOVANJE

Integrirani EU projekt BIOCOUP v okviru FP6-2004-Energy 3 z naslovom: »Co-processing of upgraded bio-liquids in standard refinery units«. Sodelujemo v podprojektu SP4 »Production of Discrete Oxygenated Target Compounds« pri identifikaciji optimalnih separacijskih strategij in tehnologij ter razvoju separacijskih tehnologij za izolacijo posameznih frakcij in diskretnih komponent.

COST Action C18, Performance assessment of

- Participation in the Centre of Excellence (coordinator Jožef Stefan Institute, Ljubljana, Slovenia), co-funded by EU-SFD, with R&D project on clean technology development in the field of selected industrial processes i.e. pure phosphoric acid/salts production, by using an integrated extraction-adsorption-desorption process.

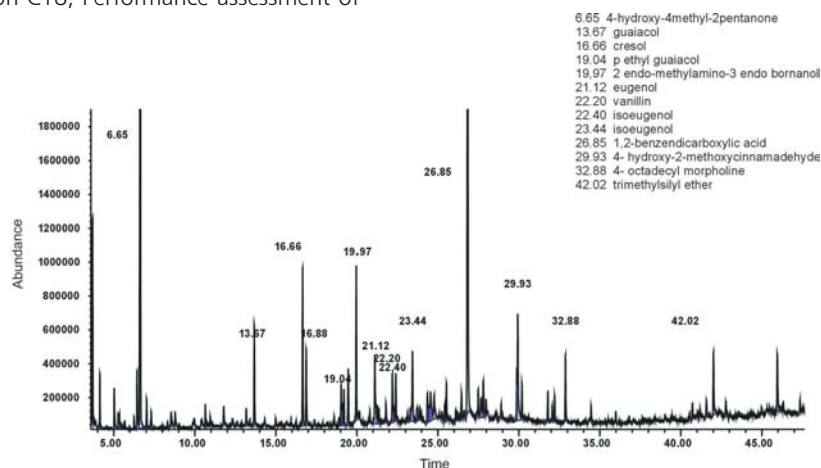
COLLABORATION WITH COMPANIES AND OTHER PARTNERS

Pilot-plant experiments, process modelling and optimization (non-catalytic chemical syntheses, component/phase separation, mixing etc.), pollution prevention and waste minimisation studies for many prominent Slovene chemical factories and process industries.

National inventories and mass balances of selected hazardous materials, environmental pollutants and wastes in order to prepare national action plans in specific fields (Ministry for environment).

IMPORTANT INSTRUMENTS AND EQUIPMENT

Laboratory of 300 m² area for pilot-scale experiments, equipped with large assortment of



SLIKA 1:

GC kromatogram dela piroliznega olja lesne biomase – surovine za razne biokemikalije

FIGURE 1:

GC of pyrolysis oil fraction, obtained from wood biomass, potential resource for basic chemicals

urban infrastructure services: The case of water supply, wastewater and solid waste. Sodelujemo v delovni skupini WG3 (trdni odpadki).

POMEMBNI INSTRUMENTI IN OPREMA

Laboratorij za pilotne kemijske poskuse (300 m²), opremljen z modularno opremo za izvajanje reakcij in separacij najrazličnejših snovnih sistemov v pilotnem oz. polindustrijskem merilu do velikosti reaktorjev 300 litrov; s pripadajočo infrastrukturo, merilno-regulacijsko opremo, računalniško programsko opremo za načrtovanje procesov ter analizo in obdelavo podatkov; oprema za določanje faznih ravnotežij tekočina-para, tekočina-tekočina in tekočina-trdno za potrebe načrtovanja separacijskih procesov, npr. destilacije, rektifikacije, ekstrakcije, absorpcije, adsorpcije, sušenja, kristalizacije ipd; programska oprema za modeliranje in vodenje procesov (ASPEN+, PARAGON, PROCEDE ...).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Obiski:

V mesecu maju 2006: obisk prof. Ralf Dohrn-a, Bayer Technology Services GmbH, Process Technology, Leverkusen, Germany in predavanje na Kemijskem inštitutu na temo »Thermophysical

modular units for carrying out chemical reactions, separations and mixing of broad range of systems in batch (up to 300 litres), semibatch and continuous mode of operation; supported by corresponding infrastructure, measuring/control equipment, personal and process computers & software; equipment for measurement and modeling of thermodynamic equilibrium of various combination of systems (liquid-vapour, liquid-liquid and liquid-solid), supporting design and calculation of basic unit operations (distillation, extraction, absorption, adsorption, drying, crystallization etc.)

EDUCATION

Supervision of student projects:

1 MSc project

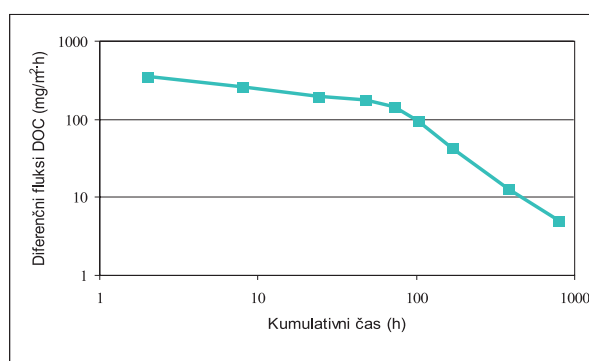
1 BSc project

Assignments:

Viktor Grilc: associate professor in chemical/environmental engineering

Ljudmila Fele Žilnik: research fellow in chemical engineering

(both at University of Ljubljana, Slovenia, Faculty for chemistry and chemical technology, lecturing regularly or by invitation on various under- and postgraduate courses in chemical and environmental engineering).



SLIKA 2:

Časovni potek izluževanja organskih snovi iz stabilizata odpadnih barv po standardnem testu EA NEN 7375. Lepo se vidi prehod iz konvekcijskega v difuzijski režim.

FIGURE 2:

Time profile of total organic compounds leaching from stabilised waste according to EA NEN 7375. Clear transition from convective to diffusional regime can be observed.

Properties for Industrial Process and Product Design«.

V mesecu aprilu: štirinajstdnevni delovni obisk
L. Fele Žilnik na Univerzi v Erlangnu, Nemčija.

Mentorstva:

1 magistrsko delo in 1 diplomsko delo na
Univerzi v Ljubljani.

Habilitacije in dejavnosti:

V. Grilc: izr. prof. za področje kemijskega in
ekološkega inženirstva (Fakulteta za kemijo in
kemijsko tehnologijo, Univerza v Ljubljani).

Poučevanje:

- Gospodarjenje z odpadnimi snovmi (Univerzitetni študij vodarstva in komunalnega inženirstva, Fakulteta za gradbeništvo in geodezijo, Univerza v Ljubljani);
- Ravnanje z odpadki (Fakulteta za gradbeništvo in geodezijo, Univerza v Ljubljani – podiplomski študij komunalne smeri) ter
- Univerza v Ljubljani – Interdisciplinarni podiplomski študij varstva okolja.

L. Fele Žilnik: znanstvena sodelavka za področje
kemijskega inženirstva (Fakulteta za kemijo in
kemijsko tehnologijo, Univerza v Ljubljani).

Poučevanje:

- gostujoča predavateljica za del predmeta Termodifuzijske operacije (Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani).

L15

Nacionalni center za NMR spektroskopijo
visoke ločljivosti - lokacija KI

National Centre for High Resolution
NMR Spectroscopy - Location NIC



VODJA / HEAD
Doc. dr. Janez Plavec

RAZISKOVALCI / RESEARCHERS

dr. Primož Šket
dr. Christophe Thibaudeau
dr. Simona Golič Grdadolnik (delno/partly)
dr. Gregor Mali (delno/partly)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Mirko Cevc
Peter Podbevšek

TEHNIČNO OSEBJE / TECHNICAL STAFF

Aleksandar Gačeša
Damjan Makuc
Gregor Ilc
Marjeta Kebrič (delno/partly)



PODROČJA DEJAVNOSTI

V program delovanja NMR centra za leto 2006 so bile vključene NMR meritve in raziskave za vse uporabnike, ki so se le te potrebovali in uporabljali pri svojem raziskovalnem in razvojnem delu v okviru osnovnih in aplikativnih raziskav in projektov za industrijo ali v industriji sami. NMR center upravlja Programski svet v sestavi: prof. dr. Janez Dolinšek (Institut Jožef Stefan, predsednik), dr. Darko Kocjan (Lek, namestnik predsednika), dr. Rok Zupet (Krka), prof. dr. Venčeslav Kaučič (Kemijski inštitut), dr. Roman Jerala (Kemijski inštitut), prof. dr. Daniel Kikelj (Fakulteta za farmacijo), dr. Mitja Kocjančič (Kmetijski inštitut Slovenije), prof. dr. Branko Stanovnik (Fakulteta za kemijo in kemijsko tehnologijo), dr. Zoran Šušterič (Sava) in dr. Simona Golič Grdadolnik (MVZT).

Program dela NMR centra za leto 2006 je obravnaval in potrdil Programski svet NMR centra. V letu 2006 je delo NMR centra potekalo v okviru vsaj 55 programov in projektov. Raziskave v okviru NMR centra so v letu 2006 izvajali raziskovalci naslednjih domačih institucij, ki so soustanoviteljice in sovlagateljice nakupa

RESEARCH ACTIVITIES

Slovenian NMR centre is a national facility open to academic researchers and researchers from industrial partners who co-financed the purchase of NMR spectrometers, as well as to the third parties which require the use of high-field high resolution NMR spectroscopy in solution or solid state in their research.

The research program for 2006 comprised NMR studies and measurements for academic institutions and researchers from industrial partners. Research program of NMR centre includes data acquisition and interpretation for those who apply NMR in their research as part of basic and applied research projects or in industry itself. Annual research program is discussed and approved by the Scientific council of NMR centre. Current members of the scientific council are: Prof. Dr. Janez Dolinšek (Institut Jožef Stefan, president), Dr. Darko Kocjan (Lek d.d., Ljubljana, Slovenia, vice president), Dr. Rok Zupet (Krka d.d., Novo mesto, Slovenia), Prof. Dr. Venčeslav Kaučič (National Institute of Chemistry), Prof. Dr. Roman Jerala (National Institute of Chemistry), Prof. Dr. Daniel Kikelj

instrumentov NMR centra: Kemijski inštitut, Institut Jožef Stefan, Fakulteta za farmacijo in Fakulteta za kemijo in kemijsko tehnologijo Univerza v Ljubljani ter Kmetijski inštitut Slovenije. V zadnjih nekaj letih smo sodelovanje NMR centra na Kemijskem inštitutu razširili na uporabnike iz Narodne in univerzitetne knjižnice Ljubljana, Inštituta za hmeljarstvo in pivovarstvo Slovenije, Naravoslovno-tehnične, Biotehniške in Medicinske fakultete Univerze v Ljubljani ter Politehniko iz Nove Gorice. Instrumenti so na razpolago vsem ustanovam in podjetjem, ki jih potrebujejo pri svojem delu. Podjetja Lek, Krka in Helios jih kot sovlagatelji pri nakupu osnovne opreme NMR centra uporabljajo pri rutinski analitiki in v okviru svojega raziskovalno razvojnega dela. V letu 2006 so instrumente v okviru NMR centra na Kemijskem inštitutu uporabljali tudi raziskovalci iz podjetij Fenolit in Kimi ter iz JRC IRMM.

Raziskave v NMR centru so obsegale:

- študij strukture oligomernih fragmentov nukleinskih kislin ter konformacijskih sprememb gradnikov DNK ob interakciji s kovinskimi ioni,
- študij strukture in dinamike proteinov, zvižanja proteinov in molekularnih interakcij peptidov z lipopolisaharidi,
- študij interakcij med ligandi in receptorjem,
- študij strukture in dinamike antibiotikov v povezavi z njihovim biološkim učinkom,
- raziskave strukture in dinamike organskih molekul, detekcija in karakterizacija reaktivnih intermediatov pri reakcijah organskih in organokovinskih spojin,
- študij naravnih produktov,
- študij sprememb v eritrocitih med bolezenskimi stanji,
- študij strukture in konformacijskih ravnotežij metabolitov v raztopini in v trdnem,
- določanje neželenih stranskih in razgradnih produktov v zdravilih,
- karakterizacijo kemijskih struktur poroznih materialov na fosfatni osnovi in strukturnih

(Faculty of Pharmacy, University of Ljubljana, Slovenia), Dr. Mitja Kocjančič (Agricultural Institute of Slovenia), Prof. Dr. Branko Stanovnik (Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia), Dr. Zoran Šušterič (Sava d.d., Kranj, Slovenia), and Dr. Simona Golič Grdadolnik (Ministry of Higher Education, Science and Technology).

In 2006 the cooperation between various research groups and NMR centre at NIC involved over 55 basic, applied and industrial projects as well as international research projects. Research was conducted by the following academic institutions that are cofounders and coinvestors into equipment of NMR centre: National Institute of Chemistry, Institute Jozef Stefan, Faculty of Pharmacy, Faculty of Chemistry and Chemical Technology (both University of Ljubljana, Slovenia) and Agricultural Institute of Slovenia. In the last few years cooperation of NMR centre at NIC has been extended to colleagues at National University Library, The Slovenian Institute for Hop Research and Brewing, Faculty of Natural Sciences and Engineering, Faculty of Biotechnology, Medicinal Faculty of University of Ljubljana, Slovenia and Polytechnic from Nova Gorica, Slovenia. Instruments are available to all institutions and companies which apply NMR spectroscopy at their work. Companies Lek d.d., Ljubljana, Slovenia; Krka d.d., Novo mesto, Slovenia and Helios d.d., Domžale, Slovenia use NMR spectrometers as analytical tool as well as in their research and development projects. In 2006 NMR centre offered services and help to companies Fenolit and Kimi as well as JRC IRMM.

Research activities of NMR centre focused on:

- structure of oligomeric nucleic acids fragments and conformational changes in DNA upon interaction with metal ions,
- protein structure and dynamics, protein folding and molecular interactions of peptides with lipopolysaharides,
- ligand-receptor interactions,
- structure and dynamics of antibiotics in rela-

- sprememb v procesu hidrotermalne sinteze zeolitov,
- študij strukture in čistosti polimernih materialov, vsebnosti stranskih produktov polimerizacije, mehanizmov polimerizacije, lastnosti polimerov z načrtovano makromolekularno strukturo,
- določanje kvalitete ter geografskega porekla slovenskih vin.

Pomemben vidik delovanja NMR centra je njegova izobraževalna vloga. NMR center nudi pomoč pri snemanju in interpretaciji NMR spektrov pri konkretnih strukturnih problemih v okviru diplomskih del, magisterijev in doktoratov.

BIBLIOGRAFIJA

- 2 izvorna znanstvena članka
- 1 samostojni znanstveni sestavek v monografiji
- 1 intervju
- 1 objavljeni znanstveni prispevek na konferenci
- 18 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 3 predavanja na tujih univerzah
- 1 vabljen predavanje na konferenci brez natisa

GLAVNI DOSEŽKI V LETU 2006

Začetek delovanja novega 800 MHz NMR spektrometra smo obeležili z mednarodnim simpozijem z naslovom "Frontiers of Biomolecular NMR – Inauguration of the 800 MHz Spectrometer & Ten Years of Slovenian NMR centre". Simpozij je potekal od 30. junija do 1. julija 2006 v Cankarjevem domu v Ljubljani. Istočasno smo obeležili deseto obletnico raziskovalnega dela na 600 MHz NMR spektrometru v okviru NMR centra na Kemijskem inštitutu. Cilj simpozija je bila izmenjava znanja in izkušenj na področju NMR spektroskopije ter neposredno povezovanje teorije in prakse.

- tion with their biological role,
- structure and dynamics of organic molecules, detection and characterization of reactive intermediates in reactions of organic and organometallic compounds,
- studies on natural products,
- studies on changes in erythrocytes during disease,
- structure and conformational equilibria of metabolites in solution and in solid state,
- determination of byproducts in pharmaceuticals,
- structural characterization of phosphate based porous materials and structural changes in the process of hydrothermal synthesis of zeolites,
- studies on structure and purity of polymers, byproducts of polymerization, mechanisms of polymerization and properties of polymers with designed macromolecular structure,
- determination of authenticity, quality and origin of Slovenian wines.

NMR centre has important role in education and training. NMR centre offers collection, and interpretation of NMR spectra on specific structural problems that are part of bachelor, masters and doctoral thesis.

BIBLIOGRAPHY

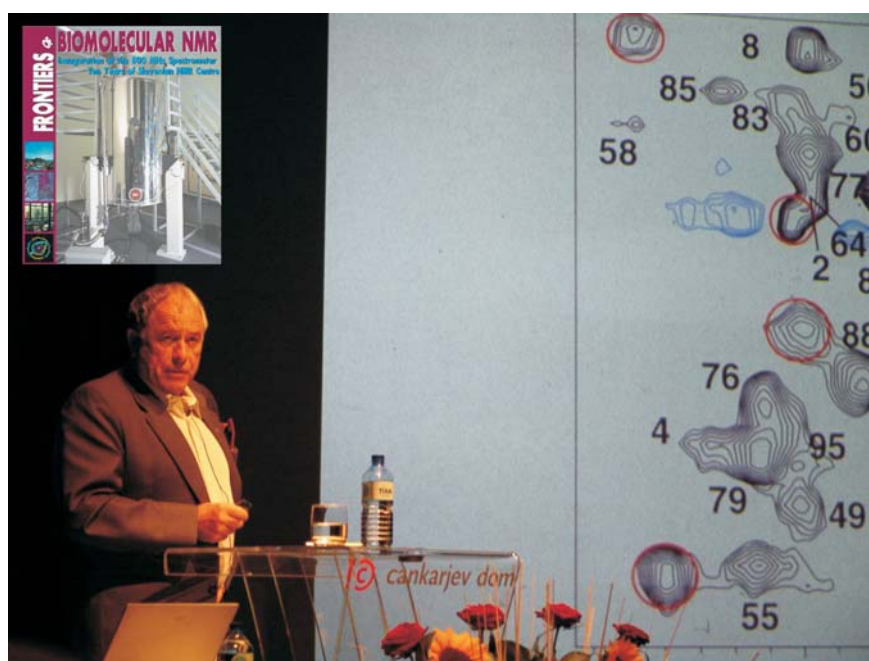
- 2 Original Scientific Articles
- 1 Independent Scientific Component Part in a Monograph
- 1 Interview
- 1 Published Scientific Conference Contribution
- 18 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 3 Invited Lectures at Foreign Universities
- 1 Invited Conference Lecture

IMPORTANT ACHIEVEMENTS IN 2006

The beginning of operation of new 800 MHz

Simpozij je ponudil pregled vseh aspektov Nuklearne Magnetne Resonance na sistemih, ki so biološko pomembni. Otvoritveno predavanje je imel Nobelov nagradjenec Kurt Wüthrich, ki je v svojem predavanju predstavil najnovejšo rezultate svojih dveh raziskovalnih skupin, in sicer na ETH v Zürichu in na Scripps Research Institute v Kaliforniji. Plenarni in ostali predavatelji, ki so se odzvali našemu vabilu, so najboljši NMR spektroskopisti v Evropi. Udeleženci iz držav Evropske unije so bili navdušeni nad kvaliteto prispevkov. Simpozij je pomenil korak k povezovanju in sodelovanju med našim NMR centrom ter slovensko industrijo, s katero sodelavci NMR centra sodelujemo in institucijami v celi Evropi. Srečanja so se udeležili tudi raziskovalci iz

NMR spectrometer was marked and celebrated through the international symposium entitled "Frontiers of Biomolecular NMR – Inauguration of the 800 MHz Spectrometer & Ten Years of Slovenian NMR centre". Symposium took place between June 30 and July 1, 2006 in Cankarjev dom, Ljubljana, Slovenia. At the same time we celebrated the tenth anniversary of research on 600 MHz NMR spectrometer. The goals of the symposium were exchange of knowledge and experience in the field of NMR spectroscopy and direct connection of theory and practice. Symposium offered an overview of all the aspects of Nuclear Magnetic Resonance on systems which are of biological relevance. The opening lecture was given by Nobel Laureate Professor Kurt Wüthrich, who has in his lecture



SLIKA 1: Profesor Kurt Wüthrich, Nobelov nagradjenec za kemijo leta 2002 je imel otvoritveno predavanje na simpoziju z naslovom "Frontiers of Biomolecular NMR – Inauguration of the 800 MHz Spectrometer & Ten Years of Slovenian NMR centre". Simpozij je potekal od 30. junija do 1. julija 2006 v Cankarjevem domu v Ljubljani

FIGURE 1: Professor Kurt Wüthrich, Nobel laureate in Chemistry in 2002 delivered an opening lecture at the symposium entitled "Frontiers of Biomolecular NMR – Inauguration of the 800 MHz Spectrometer & Ten Years of Slovenian NMR centre". Symposium took place from June 30 to July 1, 2006 in Ljubljana.

akademskih institucij in iz industrije iz Slovenije, srednje Evrope in držav članic Evropske unije. V realizacijo simpozija smo vključili tudi do- in podiplomske študente kemije, farmacije in biokemije ter raziskovalce, ki NMR spektroskopijo uporabljajo pri svojem vsakdanjem raziskovalnem ali razvojnem delu v akademskih institucijah in v industriji. Simpozij je omogočil široko platformo za izmenjavo idej, rezultatov in znanja in je vsekakor pripomogel k temu, da se slovenski raziskovalci še boljše integriramo in povezujemo z najboljšimi raziskovalnimi skupinami v Evropi.

Tematika simpozija je bila izredno pomembna tudi za raziskovalce iz farmacevtskih družb Krke in Leka, še posebno, ker sta solastniki NMR spektrometrov v okviru slovenskega NMR centra in redno uporabljata NMR spektroskopijo pri svojem delu. Med udeleženci simpozija so bili tudi sodelavci iz Heliosa, ki prav tako tesno sodelujejo z NMR centrom na lokaciji Kemijskega inštituta. Vsesplošna ocena organizatorjev, domačih udeležencev in udeležencev iz tujine je bila, da je bil simpozij izreden znanstveni dogodek in da smo začetek uporabe nove raziskovalne opreme ustrezno obeležili.

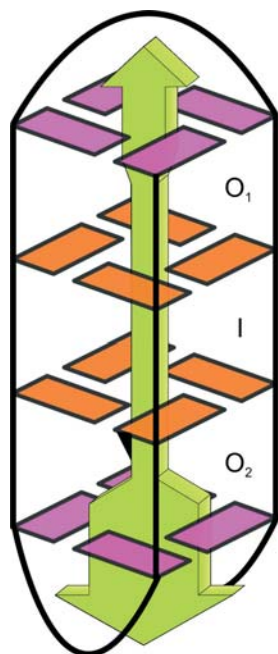
V teku je projekt Center odličnosti, pri katerem sodelujemo sodelavci Kemijskega inštituta, Leka in Krke in je sofinanciran v okviru ukrepa 1.1 Evropskega sklada za regionalni razvoj. Naslov tega ambicioznega projekta je »NMR center odličnosti za študij struktur in interakcij v biotehnologiji in farmaciji«. Raziskovalno razvojne usmeritve so zajete v 5 podsklopih oz. delovnih paketih, s katerimi fokusiramo naše aktivnosti na naslednja znanstvena in raziskovalna vprašanja, ki se zelo tesno navezujejo na konkretne probleme v farmacevtski industriji:

1. struktura in interakcije v trdnem stanju, polikristaliničnost, polimorfizem,
2. struktura in analitika organskih spojin v raztopini,
3. raziskave zmesi spojin v raztopini - profil nečistoč v zdravilih, razpadni produkti, metaboliti,

presented the latest research of his two research groups at ETH in Zürich and at Scripps Research Institute in California. Plenary and other lecturers who attended the symposium were the best NMR spectroscopists in Europe. Participants from Europe Union countries were enthusiastic about the quality of presentations. Symposium represented a step in connecting and cooperation between NMR centre and Slovene industry who are important collaborators of NMR centre and institutions all over Europe. The meeting was attended by researchers from academic institutions and from industry in Slovenia, central Europe and EU member states. Under- as well as graduate students of chemistry, pharmacy and biochemistry participated as well as researchers who apply NMR spectroscopy at their daily research and development work. Symposium represented a wide platform for exchange of ideas, results and knowledge and has certainly scientists from Slovenia to even better integrate and link with the best research groups in Europe.

Themes of the symposium were very important to researchers from slovene pharmaceutical companies Krka and Lek in particular as they have coinvested in the purchase of NMR spectrometers in Slovenian NMR centre and apply NMR spectroscopy at their work process. Among the participants were also researchers from Helios, who also closely collaborates with NMR centre at National Institute of Chemistry. General assessment of the organizers, domestic participants and participants from abroad was that symposium has been an exceptional scientific event.

The project of Centre of Excellence entitled "NMR centre of excellence for the study of structures and interactions in biotechnology and pharmacy" is running in collaboration of researchers from NIC, Lek and Krka and is co-financed by EU Structural Funds (action 1.1). Research and development orientations are divided into 5 sub-areas, or work-packages. These areas are tightly linked to problems in the pharmaceutical industry and will allow us to focus



SLIKA 2:

Shematski prikaz unimolekularnega G-kvadrupleksa, ki ga tvori oligonukleotidno zaporedje $d(G_4(T_4G_4)_3)$ v prisotnosti $^{15}\text{NH}_4^+$ ionov (na levi). G-kvadrupleks sestavljajo štiri G-kvarteti, med katerimi smo dokazali tri vezavna mesta za $^{15}\text{NH}_4^+$ ione. Ugotovili smo, da kationi niso statični, ampak se gibljejo med vezavnimi mesti in okoliško raztopino. S pomočjo 2D NzExHSQC spektrov (na desni) smo lahko določili hitrosti izmenjave $^{15}\text{NH}_4^+$ ionov skozi posamezne G-kvartete, kar shematsko ponazarjata zeleni puščici (debelejši del puščice predstavlja bolj učinkovito izmenjavo in obratno). Slika je del študije, v kateri smo P. Podbevšek, N. V. Hud (Georgia Institute of Technology, Atlanta, ZDA) in J. Plavec pokazali, da je izmenjava znotraj tega G-kvadrupleksa bistveno počasnejša kot pri bimolekularnem G-kvadrupleksu s sorodnim zaporedjem. Ugotovili smo, da je izmenjava skozi zunanja G-kvarteta hitrejša kot skozi notranja. Nadalje smo pokazali, da je razlika v hitrostih izmenjave skozi zunanja G-kvarteta posledica topologije povezovalnih T_4 zank, ki vpliva na rigidnost bližnjega G-kvarteta ter sterično ovira gibanje $^{15}\text{NH}_4^+$ ionov.

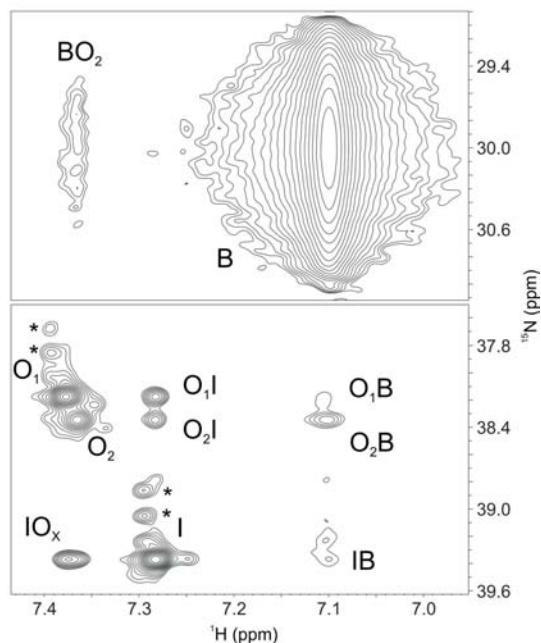


FIGURE 2:

Schematic representation of the unimolecular G-quadruplex formed by the oligonucleotide sequence $d(G_4(T_4G_4)_3)$ in the presence of $^{15}\text{NH}_4^+$ ions (on the left). G-quadruplex consists of four G-quartets and three binding sites for $^{15}\text{NH}_4^+$ ions. Bound cations are not static, but move amongst binding sites and also exchange with bulk solution. Using 2D NzExHSQC spectra (on the right) it was possible to determine the exchange rates of $^{15}\text{NH}_4^+$ ions through the individual G-quartets, which is depicted by the green arrows (broader part of the arrow indicates more efficient ion movement, and vice versa). The figure comes from the study in which P. Podbevšek, N. V. Hud (Georgia Institute of Technology, Atlanta, USA) in J. Plavec showed that the exchange within the G-quadruplex is significantly slower compared to the bimolecular G-quadruplex with a related sequence. Our data show that exchange is faster through the outer than through the inner G-quartets. Furthermore, the difference in exchange rates through the outer G-quartets shows its dependence on the topology of the connecting T_4 loops, which influence rigidity of the adjacent G-quartets and sterically hinder $^{15}\text{NH}_4^+$ ion movement.

4. karakterizacija rekombinantnih proteinov in bioloških makromolekul v raztopini,
5. interakcija zdravilnih učinkovin z biološkimi makromolekulami.

Raziskovalni dosežki, ki so nastali v sodelovanju NMR centra z raziskovalnimi laboratoriji in skupinami širom po Sloveniji, so bili objavljeni v mnogih publikacijah v revijah z mednarodnim recenzentskim sistemom (seznam je dostopen na domači strani NMR centra na naslovu www.nmr.ki.si). Precejšnje število teh dosežkov je bilo objavljenih v revijah, ki segajo v sam vrh znotraj posameznih področij znanosti. Ti dosežki bodo posebej opisani med rezultati posameznih laboratorijev na Kemijskem inštitutu ali na drugih inštitutih in fakultetah. Dosežki sodelovanja med NMR centrom in slovensko industrijo so javno znani le preko uspešnega poslovnega rezultata posameznega podjetja.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

NMR center je infrastrukturni center, ki nudi podporo najširšemu krogu akademskih in ostalih uporabnikov. Zelo intenzivni so stiki tudi z industrijskimi partnerji, ki so sovlagatelji v opremo NMR centra:

- Krka d.d., Novo mesto
- Lek d.d., Ljubljana
- Helios d.d., Domžale

Ostali uporabniki uslug NMR centra v letu 2006:

- Fenolit d.d., Borovnica
- Kimi d.o.o., Trzin

MEDNARODNO SODELOVANJE

Mednarodno sodelovanje NMR centra je obsežno (seznam mednarodnih projektov je dostopen na www.nmr.ki.si).

POMEMBNI INSTRUMENTI IN OPREMA

V okviru NMR centra na lokaciji KI so nameščeni sledeči NMR spektrometri visoke ločljivosti:

- Varian NMR systems 800
- Varian NMR systems 600

our activities on the following scientific and research questions:

1. Structure and interactions in solid state, polycrystallinity, polymorphism,
2. Structural determination and analysis of organic compounds in solution,
3. Studies of mixtures of compounds in solution - profiling of impurities in medicines, degradation products, metabolites,
4. Characterization of recombinant proteins and biological macromolecules in solution,
5. Interaction of medically active compounds with biological macromolecules.

Scientific achievements, which are the result of cooperation of NMR center with laboratories and groups around Slovenia were published in over 42 publications in journals with international peer review evaluation procedure (complete list is available on NMR center's homepage at www.nmr.ki.si). Several of these publications were published in journals which are at the top of the list within individual scientific fields. These achievements will be specifically described as results of individual laboratories at NIC or other institutes or faculties. Results of cooperation between NMR center and Slovenian industry are publicly known only through positive financial results of individual company.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

NMR centre plays a role of infrastructural facility and as such offers its support and expertise in the field of NMR spectroscopy to all interested academic research institutions as well as to commercial companies. The following industrial partners have participated in the purchase of the equipment and are regular users of NMR facility:

- Krka d.d., Novo mesto, Slovenia
- Lek d.d., Ljubljana, Slovenia
- Helios d.d., Domžale, Slovenia

- Varian Unity Inova 300
- Varian Unity Inova 300

Zadnja velika posodobitev opreme je bila izvedena s pomočjo sredstev Evropskega sklada za regionalni razvoj.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Pomemben vidik delovanja NMR centra je njegova izobraževalna vloga. NMR center nudi pomoč pri snemanju in interpretaciji NMR spektrov pri konkretnih strukturnih problemih v okviru diplomskih del, magisterijev in doktoratov.

Dr. Primož Šket je za svojo doktorsko disertacijo z naslovom "NMR študije vezave kovinskih ionov znotraj G-kvadrupleksnih struktur DNK" prejel nagrado na razpisu 36. Krkinih nagrad.

The other users of our services were:

- Fenolit d.d., Borovnica, Slovenia
- Kimi d.o.o., Trzin, Slovenia

INTERNATIONAL COLLABORATION

NMR centre is very active internationally. List of international projects is available at www.nmr.ki.si.

MAJOR EQUIPMENT

Major equipment of NMR centre includes high-resolution NMR spectrometers:

- Varian NMR systems 800
- Varian NMR systems 600
- Varian Unity Inova 300
- Varian Unity Inova 300

We are proud to note that the latest upgrade of research equipment was made possible with the financial support of EU Structural Funds.

EDUCATION AND IMPORTANT VISITS

Important aspect of NMR centre's activity is its role in educational role. NMR centre offers help at collection, and interpretation of NMR spectra on specific structural problems that are part of bachelor, masters and doctoral thesis.

Dr. Primož Šket received the prize for his Ph.D. dissertation entitled "NMR Studies of cation binding within G-quadruplex DNA structures" at the 36th Krka Awards.

L16

Center za validacijske tehnologije in
analitiko (CVTA)

Centre for Validation Technologies and
Analytics (CVTA)



VODJA / HEAD

Doc. dr. Janko Žmitek

RAZISKOVALCI / RESEARCHERS

Sodelavci iz L06 – odgovorni nosilci nalog / associates from L06:

Dr. Mirko Prošek (vodja področja / head of program)

Dr. Alenka Golc Wondra (vodja področja / head of program)

Mitja Križman

Dr. Andrej Šmidovnik

TEHNIČNO OSEBJE / TECHNICAL STAFF

Ana Andrić (začasno odsotna – porodniški dopust / temporary absence - maternity leave)

Renata Ciglarič (od / since 2. 12. 2005)

Katarina Jankovič

Adolf Krašna

Barbara Lečnik Spaić

Darija Lorber (začasno odsotna – porodniški dopust / temporary absence - maternity leave until 30. 4. 2006)

Tanja Maver (do / until 19. 7. 2006)

Katja Rožmanc Babnik



PODROČJA DEJAVNOSTI

CVTA načrtuje in izvaja razvojno-analitske storitve na področju zdravil in prehrane; njegova dejavnost obsega:

- razvoj HPLC, GC, TLC in drugih analiznih postopkov ter postopkov za določanje hitrosti raztapljanja,
- načrtovanje in izvedbo validacij analiznih postopkov,
- izvajanje analiz in analiznih študij za potrebe kontrole kakovosti izdelkov ter validacij proizvodnih tehnologij in tehnologij čiščenja proizvodne opreme,
- izvajanje analiz za študij biorazpoložljivosti oz. bioekvivalentnosti zdravil,
- validacije analiznih metod in tehnologij z navedenimi tehnikami,
- izdelavo ekspertnih mnenj in svetovanja na področju dejavnosti.

Aktivnosti potekajo v skladu s standardi dobre laboratorijske oz. dobre proizvodne prakse.

GLAVNI DOSEŽKI V LETU 2006

CVTA sledi naraščajočim potrebam slovenske in tuje farmacevtske industrije po analitski podpori

RESEARCH ACTIVITIES

CVTA designs and performs the following activities related to medicines and food:

- development of HPLC, GC, TLC, dissolution testing and other analytical procedures
- analyses and performs analytical studies for the quality control of products, and for the validation of production and cleaning technologies
- bioanalytical studies of bioavailability and bioequivalence
- validation of analytical methods and technologies
- preparation of expert opinions and consulting

Activities are performed according to GLP and/or GMP standards.

IMPORTANT ACHIEVEMENTS IN 2006

CVTA follows the increasing needs of the pharmaceutical industry for analytical support to their R&D and production projects, combined with sharpening requirements of quality standards. All the activities were performed in tight collaboration with L06, which offered profes-

razvojnim in proizvodnim projektom ob zaostrovanju kakovostnih zahtev za izvajanje takšnih del. Delo v CVTA poteka ob strokovni podpori Laboratorija za prehrabeno kemijo (L06).

V letu 2006 smo za slovensko farmacevtsko industrijo izvedli:

- razvoj dveh analitskih postopkov,
- validacijo 55 HPLC, GC in TLC analitskih postopkov,
- analize za validacijo več proizvodnih tehnologij,
- analize za validacije več tehnologij čiščenja proizvodne opreme,
- analize v okviru stabilitetnih študij za več preparatov,
- analize rezidualnih topil v ca. 600 vzorcih različnih preparatov.

Vsa dela so bila izvedena v skladu s standardi dobre laboratorijske oz. dobre proizvodne prakse.

sional support of its experts to CVTA.

Crucial achievements in the year 2006 were:

- Development of 2 analytical methods
- Validation of 55 HPLC, GC in TLC analytical methods
- Analyses for several process validations
- Analyses for several cleaning validations
- Analyses for stability studies
- Analyses of residual solvents (OVI) in approximately 600 samples of pharmaceutical finished dosage forms

All activities were performed according to GLP and/or GMP standards.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

According to the goals, CVTA has earned all its income by activities for industrial partners, particularly Lek d.d., Ljubljana, Slovenia - the member of Sandoz company, and Krka d.d., Novo mesto, Slovenia.



SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

CVTA je v skladu s cilji vse prihodke v letu 2006 ustvaril z delom za farmacevtsko industrijo, zlasti z družbama Lek d.d., Ljubljana in Krka d.d., Novo mesto.

POMEMBNI INŠTRUMENTI IN OPREMA

Več HPLC sistemov, dva GC sistema in sistem za določanje hitrosti raztapljanja ter TLC sistem (skupaj z L06). Vsi instrumenti so validirani in delujejo v skladu s principi dobre laboratorijske prakse (GLP).

MAJOR EQUIPMENT

Several HPLC systems, two GC and TLC systems, as well as a system for dissolution testing, all validated and operating according to GLP principles.

L01

Laboratorij za molekularno modeliranje in NMR spektroskopijo

Laboratory for Molecular Modelling and NMR Spectroscopy

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

1. AVBELJ, Franc, BALDWIN, Robert Lesh. Limited validity of group additivity for the folding energetics of the peptide group. *Proteins*, 2006, vol. 62, no. 2, str. 283-289. [COBISS.SI-ID 3429146]
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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

30. BRESKVAR, Matjaž, LUKMAN, Dragan, MANKOČ BORŠTNIK, Norma. On the origin of families of fermions and their mass matrices : approximate analyses of properties of four families within approach unifying spins and charges : [presented at 9th Workshop What Comes Beyond the Standard Models, Bled, September 16-26, 2006]. *Blejsk. delavn. fiz.*, 2006, letn. 7, št. 2, str. 25-50. [COBISS.SI-ID 1964132]
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Monografije in sestavki v monografijah / Monographs and Contributions in Monographs

35. DENISOV, Gleb S., MAVRI, Janez, SOBCZYK, Lucjan. Potential energy shape for the proton motion in hydrogen bonds reflected in infrared and NMR spectra. V: GRABOWSKI, Slawomir

J. (ur.). Hydrogen bonding - new insights, (Challenges and advances in computational chemistry and physics, vol. 3). Dordrecht: Springer, 2006, str. 377-416, ilustr. [COBISS.SI-ID 3637018]

Mentorstva / Mentorships

36. GROBELNIK, Barbara, Čopič, Martin (mentor), Grdadolnik, Jože (komentor). Izračun optičnih konstant v infrardečem območju z metodo oslabiljenega popolnega odboja : diplomsko delo. Ljubljana: [B. Grobelnik], 2006. 39 f., graf. prikazi. [COBISS.SI-ID 1917796]

Uredništva / Editorships

37. Journal of molecular structure. Hadži, Dušan (član uredniškega sveta 1960-). . Amsterdam: Elsevier. ISSN 0022-2860. [COBISS.SI-ID 990223]

38. Spectrochimica acta. Part A: Molecular and biomolecular spectroscopy. Hadži, Dušan (član uredniškega sveta 1995-). New York: Elsevier, 1995-. ISSN 0584-8539. [COBISS.SI-ID 26433280]

39. Acta chimica slovenica. Hadži, Dušan (član uredniškega odbora 1998-), Mavri, Janez (član uredniškega odbora 2005-). Ljubljana: Slovensko kemijsko društvo = Slovenian Chemical Society, 1993-. ISSN 1318-0207. [COBISS.SI-ID 14086149]

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Članstva v organizacijskih odborih / Memberships in Conference Committees

41. BLINC, Robert, DOLINŠEK, Janez, GOLIC GRDADOLNIK, Simona, GRIESINGER, Christian, JERALA, Roman, KAPTEIN, Robert, MALI, Gregor, PLAVEC, Janez, PRISTOVŠEK, Primož. Members of international program/organizing committee. Frontiers of biomolecular NMR - inauguration of the 800MHz spectrometer & ten years of Slovenian NMR centre. Ljubljana: Slovenian NMR Centre Ž National Institute of Chemistry, June 30 - July 1, 2006. [COBISS.SI-ID 3466266]

Intervjuji / Interviews

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L02

Laboratorij za spektroskopijo materialov

Laboratory for Spectroscopy of Materials

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

1. DULAR, Matevž, BAJCAR, Tom, SLEMENIK PERŠE, Lidija, ŽUMER, Miha, ŠIROK, Brane. Numerical simulation and experimental study of non-Newtonian mixing flow with a free surface. *Braz. J. Chem. Eng.*, 2006, letn. 23, št. 4, str. 473-486. [COBISS.SI-ID 9823259]
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5. KOVAČ, Nives, FAGANELI, Jadran, BAJT, Oliver, ŠKET, Boris, ŠURCA VUK, Angela, OREL, Boris, MOZETIČ, Patricija. Degradation and preservation of organic matter in marine macroaggregates. *Acta Chim. Slov.*, 2006, vol. 53, no. 1, str. 81-87, graf. prikazi. [COBISS.SI-ID 27487493]
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8. ŠURCA VUK, Angela, JEŠE, Robi, GABERŠČEK, Miran, OREL, Boris, DRAŽIČ, Goran. Structural and spectroelectrochemical (UV-vis and IR) studies of nanocrystalline sol-gel derived TiO₂ films. *Sol. Energy Mater. Sol. Cells.*, 2006, vol. 90, no. 4, str. 452-468. [COBISS.SI-ID 3312666]
9. TURKOVIĆ, Aleksandra, PAVLOVIĆ, Mladen, IVANDA, Mile, GABERŠČEK, Miran, CRNJAK OREL, Zorica. Influence of intercalated lithium on structural and electrical properties of V₂O₅ mixed V/Ce oxide and Fe₂O₃. *J. Electrochem. Soc.*, 2006, vol. 153, no. 1, str. A122-A126. [COBISS.SI-ID 3404570]
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14. HAUPTMAN, Nina, Jenčič, Samo (fotograf). Zeleno gorivo. *Natl. Geogr. Jr. (Ljubljana)*., april 2006, št. 28, str. 11, ilustr. [COBISS.SI-ID 3470874]

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15. CRNJAK OREL, Zorica. Characterization of novel counter electrode: mixed vanadium cerium oxides : [invited lecture]. V: HUI, David (ur.). Fourteenth annual international conference on composites/nano engineering [also] ICCE-14, July 2-8, 2006, Boulder, Colorado : [proceedings]. [S. l.: s. n.], 2006, str. 481-484. [COBISS.SI-ID 3523098]
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18. OREL, Boris, SPREIZER, Helena, ŠURCA VUK, Angela, FIR, Mojca, MERLINI, Dušan, VODLAN, Marjanca, KOHL, Michael. Optimisation of selective solar absorber paints : performance, durability and colours. V: Gleisdorf Solar 2006 - Internationales Symposium fur Sonnenenergienutzung : 6. bis 8. September 2006, Gleisdorf, Osterreich. Gleisdorf: AEE INTEC, 2006, str. 123-129. [COBISS.SI-ID 3583258]
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22. KLANJŠEK GUNDE, Marta. Actual CIE news. V: SIMONČIČ, Barbara (ur.), MOŽINA, Klementina (ur.), JELER, Slava (ur.), DEMŠAR, Andrej (ur.). 37th International Symposium on Novelties in Textiles [and] 2nd International Symposium on Novelties in Graphics [and] 7th International Symposium of SCA: Colors of National Symbols, Ljubljana, Slovenia, 15-17 June 2006. Book of proceedings. Ljubljana: Faculty of Natural Sciences and Engineering, Department of Textiles, 2006, 6 f. [COBISS.SI-ID 3502618]
23. KLANJŠEK GUNDE, Marta, GOLOB, Gorazd, AHTIK, Jure, OPARA KRAŠOVEC, Urša. Color rendering of daylight passing through switchable windows : calculations and measurements : [lecture]. V: Sixth International LRO lighting research symposium "Light and color", Orlando, Florida, February 5-8, 2006 : [proceedings]. [S. l.]: Electric Power Research Institute - EPRI, 2006, str. [1-9]. [COBISS.SI-ID 3450138]
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L03

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Laboratory of Chemometrics

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L04

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Analytical Chemistry Laboratory

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L05

Laboratorij za kemijo, biologijo in tehnologijo vod

Laboratory for Chemistry, Biology and Technology of Water

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

1. DROLC, Andreja, COTMAN, Magda, ROŠ, Milenko, MAJČEN, Nineta. Measurement traceability and its role in proficiency testing schemes - a case study for wastewater analysis in Slovenia. *Accredit. Qual. Assur.*, 2006, vol. 111, no. 8/9, str. 455-461. [COBISS.SI-ID 3472666]
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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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27. ČEPIN, Silva, Lobnik, Aleksandra (mentor), Roš, Milenko (komentor), Majcen Le Marechal, Alenka (komentor). Primerjava elektrokemijske aktivacije (ECA) in ultrazvoka pri obdelavi biocidnih odpadnih vod : magistrsko delo, (Fakulteta za strojništvo, Magistrska dela). Maribor: [S. Čepin], 2006. XVI, 131 f., ilustr. [COBISS.SI-ID 10313494]
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Uredništva / Editorships

30. European water management. Zagorc-Končan, Jana (član uredniškega odbora 1998-). Lavenham: Terence Dalton. ISSN 1461-6971. [COBISS.SI-ID 1607450]

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L06 in CVTA

Laboratorij za prehrambeno kemijo in
Center za validacijske tehnologije in analitiko (CVTA)

Laboratory for Food Chemistry and
Centre for Validation Technologies and Analytics (CVTA)

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

1. KRIŽMAN, Mitja, BARIČEVIČ, Dea, PROŠEK, Mirko. Fast quantitative determination of volatile constituents in fennel by headspace-gas chromatography. *Anal. Chim. Acta*, 2006, 557, str. 267-271. [COBISS.SI-ID 4526969]
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5. VALENTOVA, Katerina, LEBEDA, Aleš, DOLEŽALOVA, Ivana, JIROVSKY, David, SIMONOVSKA, Breda, VOVK, Irena, KOSINA, Pavel, GASMANOVA, Nikol, DZIECHCIARKOVA, Marta, ULRICHOVA, Jitka. The biological and chemical variability of Yacon. *J. Agric. Food Chem.*, 2006, vol. 54, no. 4, str. 1347-1352. [COBISS.SI-ID 3450906]
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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

7. ŽMITEK, Janko, VENTURINI, Peter. Key factors for knowledge transfer from public research : [lecture]. V: 15th international conference on management of technology [also] IAMOT 2006, May 22-26, 2006, Beijing (China). East meets west : challenges and opportunities in the era of globalization : book of abstracts [and conference proceedings]. Beijing: Tsinghua University, Research center for technological innovation, 2006, str. 173 (6 str. na CD-ROMu). [COBISS.SI-ID 3494682]

Patenti in patentne prijave / Patents and Patent Applications

8. PROŠEK, Mirko, ŠMIDOVNIK, Andrej, FIR, Maja, GOLC-WONDRA, Alenka, ŽMITEK, Janko, KOSTANJEVEC, Boštjan, DONŠA, Boštjan, VINDIŠ-ZELENKO, Brigita. Uporaba koencima Q10 za učinkovitejšo vzrejo živali in pridelavo živalskih tkiv s povečano vsebnostjo tega koencima : [slovenska patentna prijava] P-200600293, datum prijave 29.12.2006. Ljubljana: Urad RS za intelektualno lastnino, 2006. 17 str. [COBISS.SI-ID 3656986]
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Mentorstva / Mentorships

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Članstva v organizacijskih odborih / Memberships in Conference Committees

13. ERŽEN, Evgen, NOVIČ, Milko, STRLIČ, Matija, VOVK, Irena. Slovene members of international scientific committee. 12th international symposium on separation sciences, Lipica, Slovenia, September 27-29, 2006. [COBISS.SI-ID 3598874]
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L07

Laboratorij za polimerno kemijo in tehnologijo

Laboratory for Polymer Chemistry and Technology

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

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Mentorstva / Mentorships

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Članstva v organizacijskih odborih / Memberships in Conference Committees

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L08

Laboratorij za organsko sintezo in kemijo zdravil

Laboratory for Organic and Medicinal Chemistry

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

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L09

Laboratorij za anorgansko kemijo in tehnologijo

Laboratory for Inorganic Chemistry and Technology

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L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

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Članstva v organizacijskih odborih / Memberships in Conference Committees

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L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation

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Done in collaboration with the Faculty of Medicine, University of Ljubljana, Slovenia

L12

Laboratorij za biotehnologijo

Laboratory of Biotechnology

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

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L13

Laboratorij za katalizo in reakcijsko inženirstvo

Laboratory for Catalysis and Chemical Reaction Engineering

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L14

Laboratorij za procesno inženirstvo

Laboratory for Chemical Process Engineering

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14. BUČAR, Zdravko, Grilc, Viktor (mentor). Izračun emisij hlapnih organskih spojin za projekt novega vozila : diplomsko delo. Ljubljana: [M. Jeraj], 2006. 109, [4] f., ilustr. [COBISS.SI-ID 27520005]

Uredništva / Editorships

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L15

Nacionalni center za NMR spektroskopijo visoke ločljivosti - lokacija KI

National Centre for High Resolution NMR Spectroscopy - Location NIC

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

1. GAZIVODA, Tatjana, WITTINE, Karlo, LOVRIČ, Iva, MAKUC, Damjan, PLAVEC, Janez, CETINA, Mario, MRVOŠ-SERMEK, Draginja, ŠUMAN, Lidija, KRALJ, Marijeta, PAVELIČ, Krešimir, MINTAS, Mladen, RAIĆ-MALIĆ, Silvana. Synthesis, structural studies, and cytostatic evaluation of 5,6-di-O-modified L-ascorbic acid derivatives. *Carbohydr. Res.*, 2006, vol. 341, no. 4, str. 433-442, graf. prikazi. [COBISS.SI-ID 3438874]
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Članstva v organizacijskih odborih / Memberships in Conference Committees

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10. PLAVEC, Janez, Bošnjak, Dragica (oseba, ki intervjuva). Kako deluje velika biokemična tovarna - naše telo : NMR - pogled v fizikalne, kemijske in strukturne lastnosti molekul. Delo (Ljubl.), 13. jul. 2006, leto 48, št. 160, str. 18. [COBISS.SI-ID 228299008]