

Poročilo o delu 2005

Annual report 2005

POROČILO O DELU 2005 / ANNUAL REPORT 2005

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Beseda direktorja

Word of the Director



Na Kemijskem inštitutu smo jasno opredelili svoje poslanstvo in dolgoročne cilje. Osnovni cilj je visoka raven raziskav, ki edina omogoča tudi kvalitetno izobraževanje, inovativnost in dobro sodelovanje z gospodarstvom. Visoko raven raziskav pa lahko na inštitutu dosegajo vrhunski in visoko motivirani raziskovalci s sodobno raziskovalno opremo in ustreznimi pogoji za delo.

V preteklosti je bila pomembna ovira za doseganje znanstvenih dosežkov na najvišji svetovni ravni neustrezna raziskovalna infrastruktura. Težavna je bila predvsem nabava večje in dražje raziskovalne opreme za relativno majhne raziskovalne skupine. Leto 2005 je bilo posebej uspešno za inštitut pri nabavi večje raziskovalne opreme. Za uspeh je bila ključna povezava interesov več raziskovalcev in raziskovalnih skupin znotraj inštituta. Lani najpomembnejša dokončana investicija je bila nabava 800 MHz NMR spektrometra, ki je tudi največja investicija v posamezno raziskovalno opremo v Sloveniji v zadnjih letih. Nabavo novega NMR spektrometra je omogočilo odlično raziskovalno delo in dobra organiziranost NMR centra in usklajeno delovanje

At the National Institute of Chemistry, we have clearly set out our mission and long-term goals. The fundamental goal is a high level of research, which can also contribute to high-quality education, innovation, and strong cooperation with industry. A high level of research can be reached at the Institute by top-level highly motivated researchers with modern research equipment and suitable working conditions.

In the past, one of the key roadblocks to scientific achievement on a world-class level was unsuitable research infrastructure. It was difficult to acquire larger, more expensive pieces of research equipment for relatively small research groups. However, 2005 was a particularly successful year for the Institute in terms of the acquisition of larger research equipment. The key to the success of this endeavor was bringing together the interests of many researchers and research groups within the Institute. Last year the most important investment was the purchase of an 800 MHz NMR spectrometer, which was also the largest investment in an individual piece of research equipment in Slovenia in the past few years. The acquisition of the new NMR spectrometer was made possible by the excel-

mnogih inštitucij v okviru Slovenskega NMR centra ter ugled pridobljen z nazivom Evropski center odličnosti. Infrastruktura omogoča izvajanje raziskav na najaktualnejših področjih mnogim raziskovalnim skupinam na Kemijskem inštitutu ter raziskovalcem iz drugih akademskih inštitucij in podjetij.

Rezultat dela Kemijskega inštituta v letu 2005 so bile odlične znanstvene publikacije in patenti. Številni študentje so z raziskovalnim delom na inštitutu uspešno zagovarjali diplomska, magistrska in doktorska dela. Ponosni smo tudi na izdelke, ki so bili lansirani na trg v lanskem letu in so plod raziskovalnega dela sodelavcev Kemijskega inštituta. Po licenci inštituta se že izdelujejo sušilniki za tankoslojno kromatografijo in serija izdelkov z vodotopnim koencimom Q10.

Kvalitetni rezultati doseženi v preteklem letu so v veliki meri posledica vse večje mednarodne vpetosti inštituta. Velik poudarek je namenjen sodelovanju v evropskih projektih ter mobilnosti raziskovalcev. Zadovoljni smo, da zelo hitro raste število kvalitetnih tujih znanstvenikov, ki opravljajo raziskave na Kemijskem inštitutu. Za inštitut je izrednega pomena tudi tradicionalno zelo dobra povezanost s slovenskimi podjetji, pomembno pa se je okrepilo tudi sodelovanje s številnimi podjetji po svetu. Pričakujemo, da se bo sodelovanje s podjetji v tujini v prihodnje še povečalo preko podjetja VICIM, ki smo ga na Nizozemskem ustanovili skupaj s našimi partnerji.

Tudi vnaprej si bomo prizadevali zagotoviti kvalitetne pogoje dela in kvalitetno raziskovalno opremo najboljšim raziskovalcem. Zaradi velike prostorske stiske smo v letu 2005 pričeli z aktivnostmi za pridobitev novih delovnih površin na obstoječi lokaciji. Dolgoročni cilj pa ostaja postavitev novega objekta inštituta na primernejši lokaciji. Naš prispevek želimo v prihodnje povečati pri izobraževanju, kjer se odpirajo možnosti aktivnejše vloge inštituta. Še bolj bomo vzpodbujali tudi inovativnost in krepili naš prispevek pri gospodarskem napredku.

lent research work and strong organization of the NMR center, the combined efforts of many institutions within the framework of the Slovenian NMR center, and the respect earned by being named a European Center of Excellence. Investment in infrastructure allows research groups at the National Institute of Chemistry and researchers from other academic institutions, as well as companies, to carry out research in the most up-to-date fields.

The results of the work of the National Institute of Chemistry in 2005 were excellent scientific papers and patents. In addition, a number of students completed their undergraduate, master's, and doctoral degrees through their research work at the Institute. We are also proud of the products which were launched onto the market and are the fruit of research work carried out by members of the Institute. Dryers for thin layer chromatography and a series of products using water-soluble coenzyme Q10 are being produced under license from the Institute.

The quality of the results achieved in the past year is to large extent the result of the increased international involvement of the Institute. A large emphasis has been placed on cooperation in European projects and the mobility of researchers. We are pleased with the quick growth in the number of high-quality foreign scientists carrying out research at the National Institute of Chemistry. For the Institute, it is still of exceptional importance to maintain the traditionally strong ties with Slovenian companies, as well as to strengthen cooperation with companies around the world. We expect that cooperation with foreign companies will increase in the future through the company VICIM, which the Institute founded in the Netherlands together with our partners.

We will continue to work on ensuring good working conditions and high-quality research equipment to our best researchers. In 2005, we also undertook to increase the workspace available at our current location, as space is

Prepričan sem, da bomo zastavljene cilje uresničili s skupnimi naporima vseh sodelavcev inštituta ter s sodelovanjem z našimi partnerji v akademskih inštitucijah, gospodarstvu in drugod.

extremely limited; however the longer term goal is a new building for the Institute at a better location. We would like to increase our contribution in the sphere of education in the future, where possibilities for an active role of the Institute are opening up. We will continue to encourage innovation and to strengthen our contribution to Slovenia in terms of economic advancement.

I am certain that the stated goals can be realized with a concerted effort of all our colleagues at the Institute and with the cooperation of partners in academic institutions, industry, and elsewhere.

Pel Va L
doc. dr. Peter Venturini



SLIKA:

Evropski komisar za znanost in raziskave dr. Janez Potočnik, direktor Kemijskega inštituta dr. Peter Venturini in slovenski minister za visoko šolstvo, znanost in tehnologijo dr. Jure Zupan so odprli nove raziskovalne zmogljivosti na Kemijskem inštitutu (29. 10. 2005).

FIGURE:

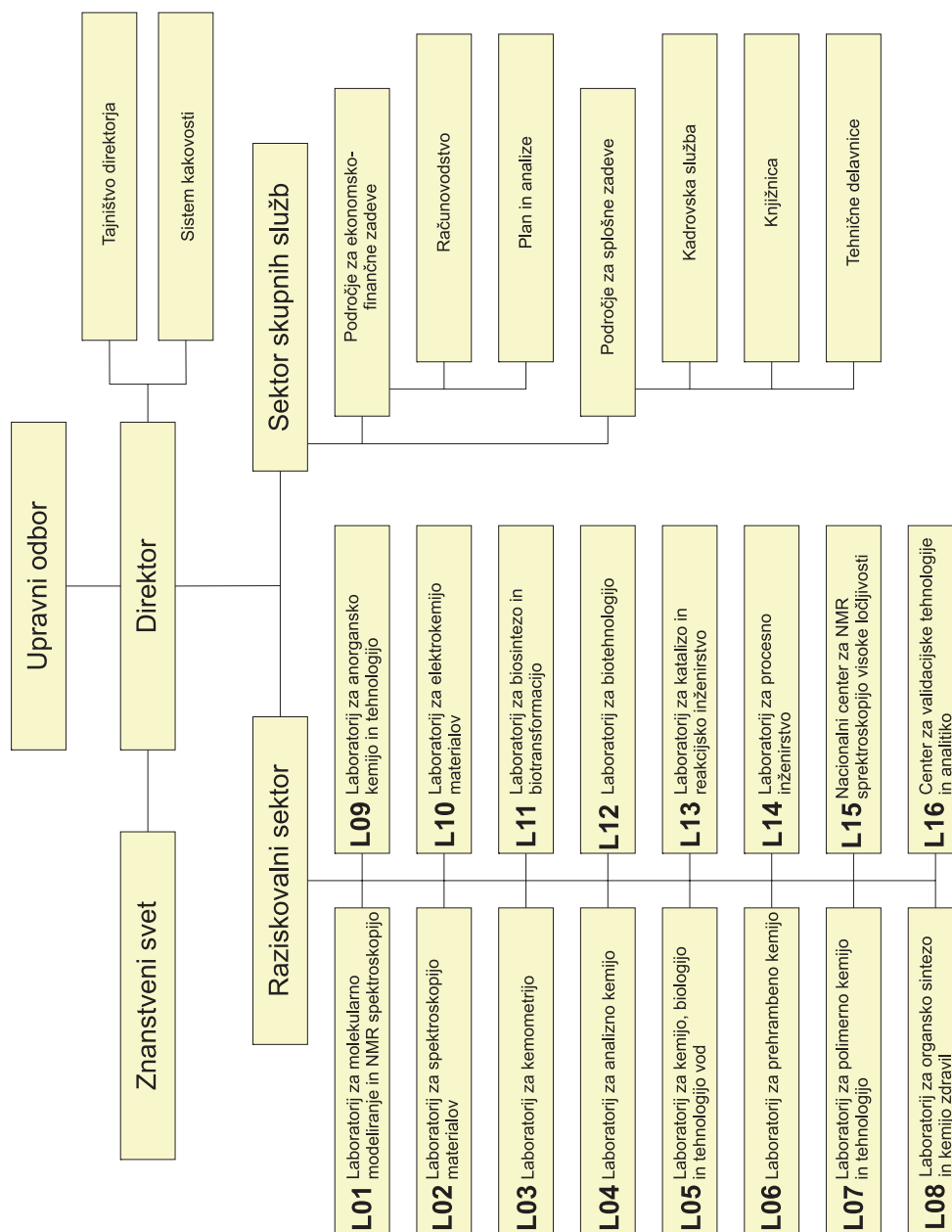
The European Commissioner for Science and Research Dr. Janez Potočnik, the Director of the National Institute of Chemistry Dr. Peter Venturini, and the Slovenian Minister for higher Education, Science and Technology Dr. Jure Zupan opened new research facilities at the National Institute of Chemistry. (29. 10. 2005).

Poslanstvo Kemijskega inštituta

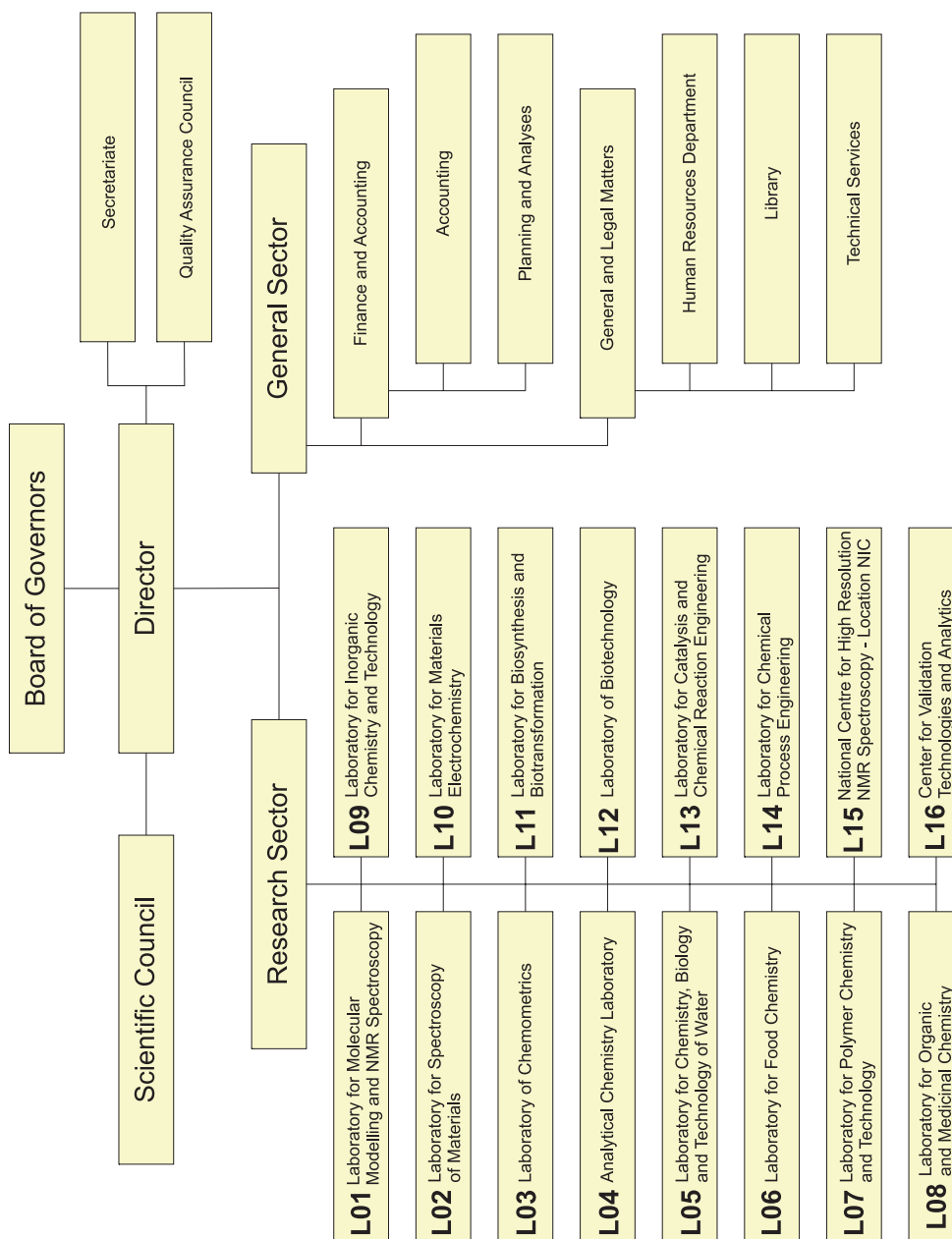
The Mission of the National Institute of Chemistry

- 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

- **Pomočnika direktorja /
Assistant directors**

Mag. Janez TOPLIŠEK

Mag. Renata VUGA

- **Svetovalec direktorja /
Councillor to the director**

Doc. dr. Janko ŽMITEK

ČLANI UPRAVNEGA ODBORA / BOARD OF GOVERNORS

- Dr. Stojan Sorčan, predsednik / president (do / until 2. 3. 2005)
- Dr. Zvonko Bergant (od / since 3. 3. 2005)
- Dr. Ilija Dimitrievski (do / until 2. 3. 2005)
- Akad. prof. dr. Dušan Hadži
- Prof. dr. Roman Jerala
- Prof. dr. Julijana Kristl (od / since 3. 3. 2005)
- Dr. Andrej Kržan
- Prof. dr. Ivan Leban (do / until 13. 11. 2005)
- Dr. Brina Ornik
- Dr. Matej Penca (od / since 3. 3. 2005)
- Doc. dr. Janez Plavec
- Dr. Aleš Rotar (do / until 2. 3. 2005)
- Dr. Tomaž Šolmajer (od / since 3. 3. 2005)

ČLANI ZNANSTVENEGA SVETA / SCIENTIFIC COUNCIL

- Akad. prof. dr. Janez Levec, predsednik / president (do / until 13. 12. 2005)

- Doc. dr. Janko Jamnik predsednik / president (od / since 14. 12. 2005)
- Dr. Franc Avbelj (od / since 14. 12. 2005)
- Prof. dr. Branko Borštnik (od / since 14. 12. 2005)
- Prof. dr. Roman Jerala (od / since 14. 12. 2005)
- Prof. dr. Venčeslav Kaučič
- Prof. dr. Radovan Komel (do / until 13. 12. 2005)
- Doc. dr. Janez Mavri (do / until 13. 12. 2005)
- Dr. Marjana Novič (do / until 13. 12. 2005)
- Dr. Albin Pintar (od / since 14. 12. 2005)
- Doc. dr. Janez Plavec
- Dr. Mirko Prošek (do / until 13. 12. 2005)
- Prof. dr. Milenko Roš
- Izr. prof. dr. Majda Žigon (od / since 14. 12. 2005)
- 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)

	2005	2004	Struktura 2005 (%)	Indeks 2005/2004
Raziskovalni programi	856.648	835.312	35	103
Infrastrukturni programi	97.950	99.539	4	98
Raziskovalni projekti	289.270	272.827	11	106
Ustanoviteljske obveznosti	408.295	392.287	16	104
Mladi raziskovalci	241.720	198.729	8	122
Domači trg	454.089	399.857	17	114
Tuji trg	125.495	124.843	5	101
Drugi prihodki	115.206	81.129	4	142
SKUPAJ PRIHODKI	2.588.673	2.404.523	100	108

ODHODKI (1000 SIT)

	2005	2004	Struktura 2005 (%)	Indeks 2005/2004
Stroški materiala	-278.473	-247.922	11	112
Stroški storitev	-356.006	-317.147	14	112
Amortizacija	-249.974	-230.183	10	109
Stroški dela	-1.512.741	-1.459.714	63	104
Drugi odhodki	-30.890	-61.953	2	50
SKUPAJ ODHODKI	-2.428.084	-2.316.919	100	105

REZULTAT POSLOVANJA	160.589	87.604	-	183
----------------------------	----------------	---------------	----------	------------

Finances

REVENUES (1000 SIT)

	2005	2004	Structure 2005 (%)	Index 2005/2004
Research programmes	856.648	835.312	35	103
Infrastructure programmes	97.950	99.539	4	98
Research projects	289.270	272.827	11	106
Overhead financing	408.295	392.287	16	104
Young researchers	241.720	198.729	8	122
Domestic market	454.089	399.857	17	114
Foreign market	125.495	124.843	5	101
Other incomes	115.206	81.129	4	142
TOTAL	2.588.673	2.404.523	100	108

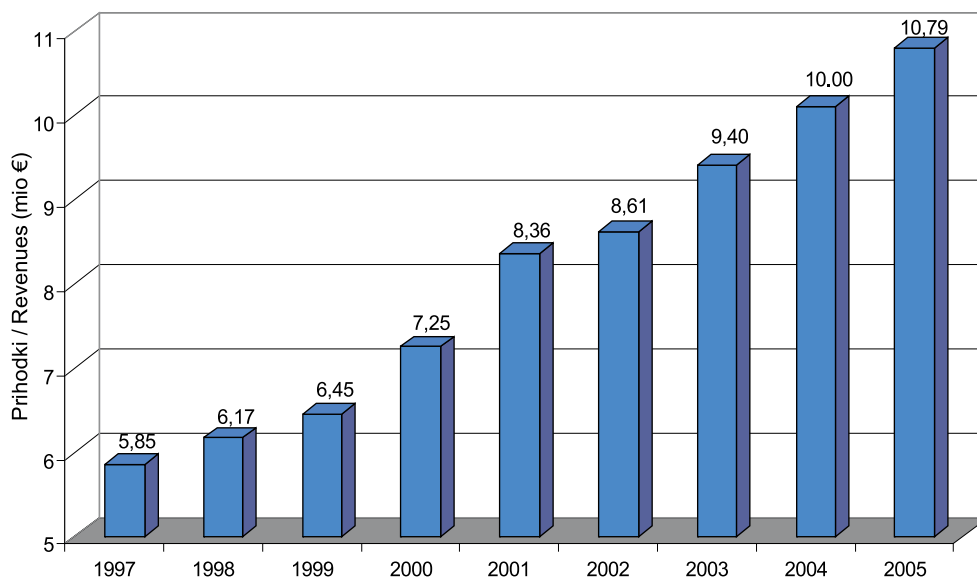
OUTFLOW (1000 SIT)

	2005	2004	Structure 2005 (%)	Index 2005/2004
Costs of material	-278.473	-247.922	11	112
Costs of services	-356.006	-317.147	14	112
Depreciation	-249.974	-230.183	10	109
Labour costs	-1.512.741	-1.459.714	63	104
Other outcomes	-30.890	-61.953	2	50
TOTAL	-2.428.084	-2.316.919	100	105

FINAL RESULT	160.589	87.604	-	183
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Prihodki Kemijskega inštituta

Revenues of the National Institute of Chemistry



SLIKA

Prihodki Kemijskega inštituta v mio EUR.

FIGURE

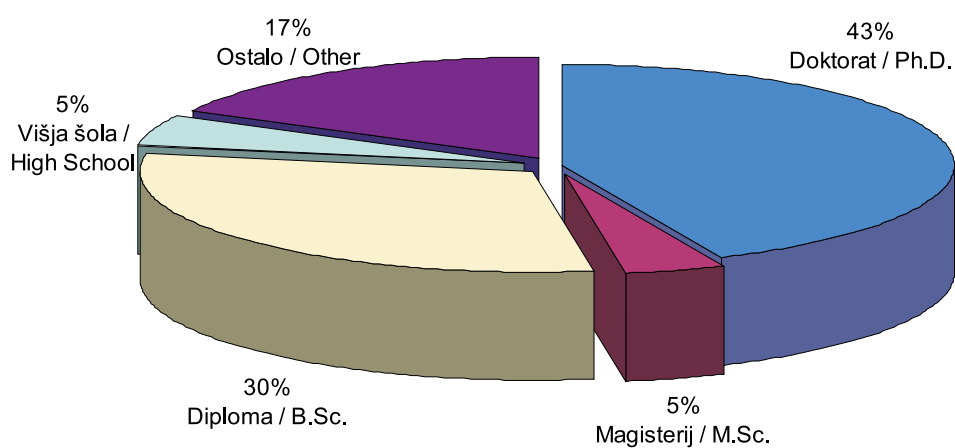
Revenues of the National Institute of Chemistry in million euros.

Zaposleni

Personnel

Na dan 31. 12. 2005 je bilo na Kemijskem inštitutu 227 zaposlenih, od tega 97 doktorjev znanosti, 10 magistrov, 69 z visoko izobrazbo, 12 z višjo izobrazbo, 29 s srednjo in 10 z nižjo izobrazbo. Število zaposlenih se je glede na predhodno leto povečalo za 8 %, predvsem na račun uspešnih prijav na razpis za mlade raziskovalce.

On December 31, 2005, we have recorded 227 employees with the following degree of education: Ph.D. (97), Master degree (10), Bachelor degree (69), Associate degree (12), secondary school (29) and less than secondary school (10). Compared to the previous year the number of employees rose by 8 %, mainly due to a number of successful applications for the "Young Researcher" tender.



SLIKA
Izobrazbena struktura zaposlenih na Kemijskem inštitutu v letu 2005.

FIGURE
Employees level of education at the National Institute of Chemistry in 2005.

Doktorati, magisteriji in diplome v letu 2005

Doctoral, Master's and Graduate Theses in Year 2005

DOKTORATI / DOCTORAL THESES

- Apolonija Bedina Zavec, 4. 10. 2005
- Irena Fonda, 26. 5. 2005
- Brigita Lapornik, 26. 5. 2005
- Mateja Manček Keber, 4. 4. 2005
- Mojca Merhar, 13. 5. 2005
- Miha Plevnik, 28. 6. 2005

- Alanka Ristić, 9. 6. 2005

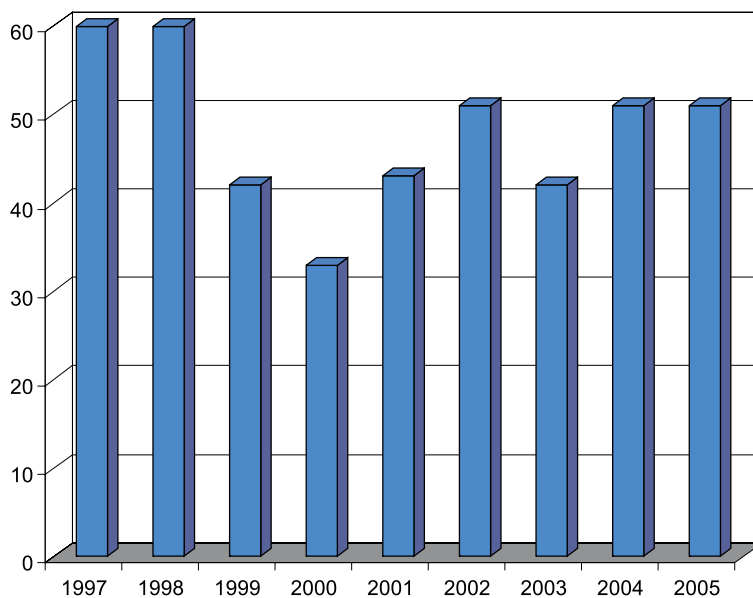
- Monika Stražičar, 6. 4. 2005

- Primož Šket, 21. 12. 2005

- Matevž Vospernik, 6. 7. 2005

MAGISTERIJI / MASTER'S THESES

- Nada Verdel, 10. 2. 2005



SLIKA

Doktorati, magisteriji in diplome v letih
1997 / 2005.

FIGURE

Ph.D., M.Sc., and B.Sc. theses in years
1997 / 2005.

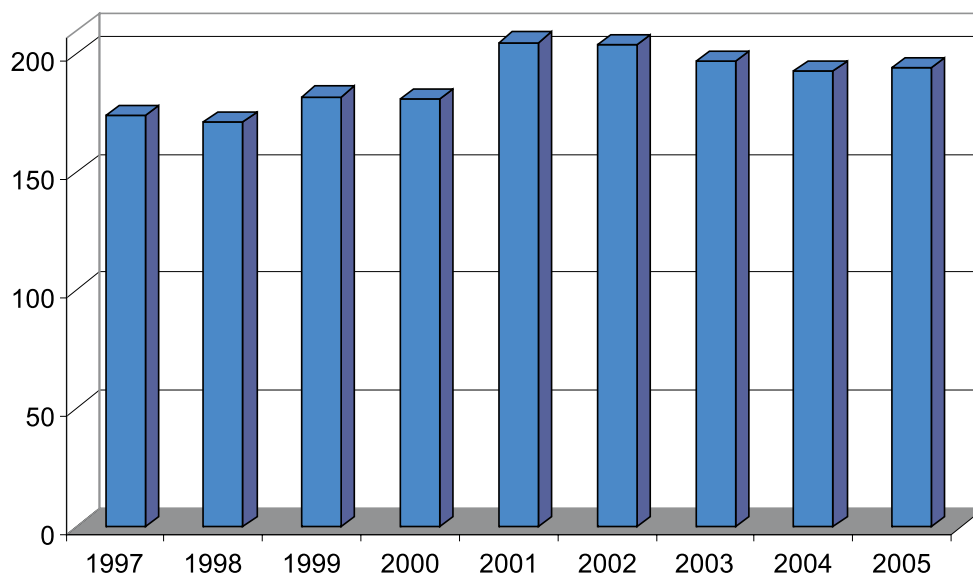
**ŠTEVILO DIPLOM, MAGISTERIJEV, DOKTORATOV, MENTORSTEV IN KOMENTORSTEV S
STRANI ZAPOSLENIH NA KEMIJSKEM INŠTITUTU**

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

2	diplomski deli / Undergraduate Theses
1	magistrsko delo / Master's Thesis
10	doktorskih disertacij / Doctoral Theses
9	mentorstev pri diplomskih delih / Mentorships of Undergraduate Theses
2	mentorstvi pri magistrskih delih / Mentorships of Master's Theses
1	mentorstvo pri doktorski disertaciji / Mentorship of Doctoral Thesis
24	komentorstev pri diplomskih delih / Comentorships of Undergraduate Theses
3	komentorstva pri magistrskih delih / Comentorships of Master's Theses
1	komentorstvo pri doktorski disertaciji / Comentorship of Doctoral Thesis

Objave v letu 2005

Published Works in Year 2005



SLIKA
Objavljena dela (članki, knjige, poglavja, patenti) v letih 1997 / 2005.

FIGURE
Published works (papers, books, chapters, patents) in years 1997 / 2005.

Bibliografija inštituta v letu 2005
ANALITIČNI PODATKI (tipologija COBISS /
laboratoriji)

Institute bibliography for 2005
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	35	34	23	17	12	11	23	3	11	13	15	20	10	2	6	235	11	224
Prispevki na konferencah / Conference contributions	48	44	26	41	33	19	42	2	21	21	34	26	12	11	17	397	29	368
Patenti / Patents	0	0	0	0	0	3	2	3	0	1	8	2	1	0	0	20	0	20
Predavanja / Lectures	7	2	2	1	5	0	10	1	3	0	2	6	0	2	3	44	0	44
Dokumenti / Documents	4	1	0	10	13	2	2	0	1	6	0	0	3	14	0	56	3	53
Doktorati, magisteriji, diplome / PhD, MSc, BSc	2	3	1	0	4	9	5	2	1	2	6	9	2	3	3	52	1	51
SKUPAJ / ALL UNITS	96	84	52	69	67	44	84	11	37	43	65	63	28	32	29	804	44	760

Mednarodno sodelovanje

International Cooperation

MULTILATERALNO SODELOVANJE / MULTILATERAL COOPERATION	
5. Okvirni program EU / 5th Framework Programme EU	5
6. Okvirni program EU / 6th Framework Programme EU	8
COST	5
PROTEUS	4
Skupno / Total	22

BILATERALNO SODELOVANJE / BILATERAL COOPERATION	
Avstrija / Austria	1
Češka / Czech Republic	3
Hrvaška / Croatia	7
Indija / India	3
Italija / Italy	3
Madžarska / Hungary	2
Makedonija / Macedonia	1
Nemčija / Germany	1
Poljska / Poland	1
Portugalska / Portugal	1
Romunija / Romania	1
Srbija in Črna gora / Serbia and Montenegro	3
Turčija / Turkey	1
Velika Britanija / Great Britain	7
ZDA / USA	3
Skupno / Total	38

Nagrade podeljene sodelavcem inštituta v letu 2005

Awards Given To Collaborators with the Institute in 2005

Nagrada Kemijskega inštituta za izjemno doktorsko delo, 8. 12. 2005

podeljena najboljšim med raziskovalci, ki so na Kemijskem inštitutu v preteklem obdobju zaključili raziskovalno delo za doktorsko disertacijo:

- **Dr. Mateja Manček Keber:** LPS-vezavni proteini: analiza lastnosti in interakcij z endotoksinom; mentor: prof. dr. Roman Jerala
- **Dr. Jernej Stare:** Dinamika in struktura sistemov s kratkimi vodikovimi vezmi; mentorja: akad. prof. dr. Dušan Hadži, doc. dr. Janez Mavri

35. Krkine nagrade 2005, Novo mesto, 28. 10. 2005:

- **Dr. Miha Plevnik:** Strukturne raziskave predorganizacije prostorskih struktur oligomernih nukleinskih kislin; doktorska disertacija, Krkina nagrada za posebne dosežke, mentor: doc. dr. Janez Plavec
- **Dr. Mateja Manček Keber:** LPS-vezavni proteini: analiza lastnosti in interakcij z endotoksinom; doktorska disertacija, mentor: prof. dr. Roman Jerala
- **Dr. Marko Oblak:** Strukturno podprto načrtovanje novih inhibitorjev DNA giraz z

The National Institute of Chemistry Award for Exceptional Doctoral Work, 8. 12. 2005

awarded to the best researchers, that recently completed their doctoral research work at The National Institute of Chemistry:

- **Dr. Mateja Manček Keber:** LPS binding proteins: analysis of their properties and interactions with endotoxin; mentor: Prof. Dr. Roman Jerala
- **Dr. Jernej Stare:** Structure and dynamics of the systems with short hydrogen bonds; mentors: Prof. Dr. Dušan Hadži, Dr. Janez Mavri

35th Annual Krka Prizes, Novo mesto, Slovenia; October 28, 2005:

- **Dr. Miha Plevnik:** Structural Studies of Preorganization of 3D Structures of Oligomeric Nucleic Acids; doctoral dissertation, Krka Prize for Special Achievements in Research, mentor: Dr. Janez Plavec
- **Dr. Mateja Manček Keber:** LPS binding proteins: analysis of their properties and interactions with endotoxin; doctoral dissertation, mentor: Prof. Dr. Roman Jerala
- **Dr. Marko Oblak:** Structure based drug design of novel ATPase inhibitors of the DNA gyrase; doctoral dissertation, mentor: Prof. Dr. Tomaž Šolmajer

delovanjem na ATP-vezavnem mestu; doktorska disertacija, mentor: izr. prof. dr. Tomaž Šolmajer

Prešernove nagrade študentom Univerze v Ljubljani, 29. 11. 2005:

- **Alen Kljajić:** Novi mezoporozni materiali na silikatni osnovi; raziskovalna naloga, mentor: prof. dr. Venčeslav Kaučič

Prešernove nagrade študentom Fakultete za farmacijo, Univerza v Ljubljani, 30. 11. 2005:

- **Aljaž Godec in Uroš Maver:** Stabilizacija amorfnega nifedipina v kserogelu SiO₂; diplomska naloga, somentor: dr. Marjan Bele

Prešeren Prize of University of Ljubljana, Slovenia; November 29, 2005:

- **Alen Kljajić:** Novel silicate-based mesoporous materials; Undergraduate Thesis, mentor: Prof. Dr. Venčeslav Kaučič

Faculty Prešeren Prize presented by the Faculty of Pharmacy of the University of Ljubljana, Slovenia, for Undergraduate Thesis Work; November 30, 2005:

- **Aljaž Godec in Uroš Maver:** Stabilization of amorphous nifedipine in a SiO₂ xerogel; comentor: Dr. Marjan Bele



SLIKA:

Podelitev nagrad za izjemno doktorsko delo. Od leve proti desni: predsednik Znanstvenega sveta prof. dr. Janez Levec, ga. Branka Stare - mama nagrajenca dr. Jerneja Stareta, direktor dr. Peter Venturini, nagrajenka dr. Mateja Manček Keber in predsednik komisije za nagrado Kemijskega inštituta za izjemno doktorsko delo dr. Franc Avbelj

FIGURE:

Awarding of prizes for exceptional doctoral work. From left to right: President of the Science Council Prof. Dr. Janez Levec, Mrs. Branka Stare – mother of prizewinner Dr. Jernej Stare, director Dr. Peter Venturini, prizewinner Dr. Mateja Manček Keber, and President of the award commission of the National Institute of Chemistry for exceptional doctoral work Dr. Franc Avbelj (8. 12. 2005).

Prešernove nagrade študentom Fakultete za kemijo in kemijsko tehnologijo, Univerza v Ljubljani, 23. 11. 2005:

- **Jure Hren:** Asimetrično hidrogeniranje iminov s prenosom vodika, diplomska naloga, somentor: dr. Barbara Mohar
- **Lea Mauko:** Izdelava in preizkus mikroelektrode za določanje pH papirja umetnostno - zgodovinske vrednosti; diplomska naloga, mentor: doc. dr. Matija Strlič

Faculty Prešeren Prize presented by the Faculty of Chemistry and Chemical Technology of the University of Ljubljana, Slovenia for Undergraduate Thesis Work; November 23, 2005:

- **Jure Hren:** Asymmetric transfer hydrogenation of imines; comentor: Dr. Barbara Mohar
- **Lea Mauko:** Making and testing microelectrode for pH determination of paper of artistic and historical value; mentor: Dr. Matija Strlič

Zaposleni v splošnem sektorju

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Zdenka Laznik

ŠTIPENDIJE / SCOLARSHIPS

Alen Kljajić
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
Prof. dr. Adolf Miklavc
Dr. Ksenija Poljanec
Dr. Matej Praprotnik
Dr. Danilo Pumpernik
Dr. Jernej Stare
Prof. dr. Tomaž Šolmajer
Dr. Gregor Mlinšek

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Urban Borštnik
Urban Bren
Janez Konc
Tjaša Urbič
Jernej Zidar

TEHNIČNO OSEBJE / TECHNICAL STAFF

Tatjana Karba
Silva Zagorc

PRIPRAVNIKI / TRAINEES

Borut Tone Oblak
Špela Klofutar



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 biomolekularna 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 medmolekularskih 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

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 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

J1-5115 **(F. Merzel)**

Simulations and structural analysis of water at protein surfaces

dinamike, analize po normalnih načinih nihanja in kvaziharmonske analize proteinov v raztopinah za študij hidratacije proteinov

- Razvoj in uporaba QM/MM metod
- 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 računske gruče

BIBLIOGRAFIJA

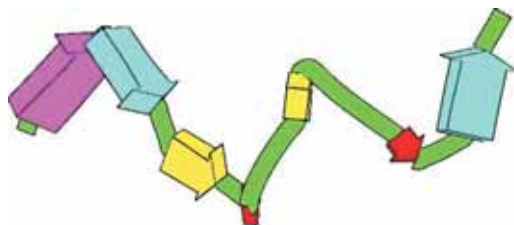
- 31 izvirnih znanstvenih člankov
- 1 kratki znanstveni prispevek
- 1 samostojni znanstveni sestavek v monografiji
- 2 drugi učni gradivi
- 4 objavljeni znanstveni prispevki na konferencah (vabljeni predavanja)
- 7 objavljenih znanstvenih prispevkov na konferencah
- 36 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 4 predavanja na tujih univerzah
- 2 prispevka na konferencah brez natisa
- 1 vabljeni predavanje na konferenci brez natisa

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
- 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

- 31 Original Scientific Articles
- 1 Review Article
- 1 Independent Scientific Component Part in a Monograph
- 2 Other Educational Material
- 4 Published Scientific Conference Contributions (Invited Lecture)
- 7 Published Scientific Conference Contributions



SLIKA 1:

Fleksibilni beta-trakovi v kemično denaturiranem ubikvitinu (8M urea)

FIGURE 1:

Fluctuating beta-strands in chemically denatured ubiquitin (8M urea)

- 1 elaborat, predštudija, študija
- 3 končna poročila o rezultatih raziskav
- 1 diploma
- 1 magisterij
- 4 uredništva revij

GLAVNI DOSEŽKI V LETU 2005

- Z eksperimentalnimi in teoretskimi metodami smo ugotovili, da so konformacijske preference aminokislin, blokiranih s $\text{CH}_3\text{CO-}$ in $-\text{NH-CH}_3$ skupinami (dipeptidi), enake preferencam amino kislinskih ostankov v majhnih peptidih in v tistih segmentih proteinov, ki ne tvorijo α -vijačnic ali β -plasti. Takšno obnašanje dipeptidov je v skladu z našim teoretskim modelom, v katerem elektrostatsko senčenje določa lokalno strukturo peptidov in proteinov. Ugotovili smo tudi, da princip aditivnosti, ki se standardno uporablja pri študiju energetike proteinov, ne velja za peptidno skupino. S pomočjo računalniških simulacij smo ugotavljali stabilnost krajših fragmentov proteina G. Naš cilj je bil ugotoviti, kako dolg mora biti peptid, da je stabilen in ima zvitje podobno nativnemu. Rezultati so pokazali, da konformacijska entropija narašča od fragmenta s štirimi, do fragmenta s sedmimi amino kislinami in nato pada do fragmenta z 11 amino kislinami. Struktura fragmentov, katerih dolžina se približuje 11 amino kislinam, postaja podobna nativni obliki.
- Študirali smo konformacijske lastnosti steroidnega estra, ki ima visoko biološko aktivnost in nizko toksičnost in predstavlja prototip za razvoj serije novih učinkovin z močnim anti-rakotvornim delovanjem. Rezultati kažejo, da je preferenčna orientacija alkilne verige molekule odvisna od konfiguracije steroidnega skeleta in povezana z mehanizmom anti-rakotvornega delovanja. Znano je, da majhne kemijske spremembe steroidnega dela močno vplivajo na anti-rakotvorno aktivnost teh spojin.
- Časovni potek protonsko-devterijeve izmenjave v trdnem proteinu smo spremljali z IR spektroskopijo. Z uporabo diferenčne

- 36 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 4 Invited Lectures at Foreign Universities
- 2 Unpublished Conference Contributions
- 1 Unpublished Invited Conference Lecture
- 1 Treatise, Preliminary Study, Study
- 3 Final Research Reports
- 1 Undergraduate Thesis
- 1 Master's Thesis
- 4 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2005

- Using experimental and theoretical methods we have shown that the backbone conformational preferences, displayed by amino acid residues in peptides and by residues outside repetitive secondary structures (α -helices, β -sheets) in proteins, are fully present in dipeptides (amino acids blocked by $\text{CH}_3\text{CO-}$ and $-\text{NH-CH}_3$ groups). Such behavior is in accord with our theoretical model in which electrostatic screening determines local structures of peptides and proteins. We also found that the group additivity principle, which is a standard feature of analyses of the energetics of protein folding, is not valid for peptide groups. We have performed all-atom computer simulations on short peptide fragments of G protein. Our goal was to find the optimal length of a fragment that is stable and also resembles the native state. The results show that the conformational entropy increases from fragment with 4 amino acids to the one with 7 amino acids and then decreases to the fragment with 11 amino acids. We found that as the fragment approaches 11 monomer units the structures begin to converge to a native-like structure.
- We investigated conformational properties of steroidal ester, which has high biological activity and low toxicity and serves as a prototype for design of novel potent anti-tumor agents. Our results indicate that the preferences in the orientation of the alkyl chain are

spektroskopije, metode spektralne dekompozicije in Laplace-ove transformacije smo določili konstante izmenjave za posamezne dele proteina. Ugotovili smo, da je hitrost izmenjave odvisna od sekundarne strukture in izpostavljenosti toplu. Z analizo amidnega I traku v infrardečem spektru proteina smo pokazali, da metoda, ki so jo predlagali sodelavci, ekstrahira pravilno zviti protein. Pokazali smo tudi, da ATR spektroskopija z izračunanimi optičnimi konstantami omogoča *in-situ* spremljanje kemijskih oz. elektrokemijskih reakcij. Z uporabo ATR spektroskopije in z izračunanimi absorpcijskimi spektri smo razložili vpliv vodikovih vezi na tvorjenje razvejanih poliestrov.

- Vloga dinamike protonov v vodikovih vezeh z bolj ali manj simetričnim potencialom z dvema minimi narekuje študij modelnih sistemov in vpliva okolice na potenciale ter pretek teh na dinamiko. Med najbolj informativne pristope sodijo vibracijske spektroskopije oprte na računalniško modeliranje. Za modelne sisteme smo izbrali N-oksidi substituiranih pikolinskih kislin, ker efekti substituent vodijo v variacije jakosti vodikovih vezi, ki pa so tudi zelo občutljive na učinke okolice. Druga serija modelnih spojin so β -enoloni. Poleg tega, da igrata vlogo modelnih sistemov, sta obe seriji zanimivi tudi zaradi nasprotij v interpretaciji infrardečih spektrov, ki nastopajo v literaturi že vsaj 30 let, jih je pa treba razrešiti za polno izkoriščanje informacij, ki so vsebovane v spektrih. Prvi rezultati so bili objavljeni leta 2000. Opisana je bila analiza infrardečega spektra N-oksida pikolinske kisline v argonski matriki. Delo zahteva uporabo eksperimentalnih metod, ki pri nas niso dostopne (infrardeči spektri v matriki žlahtnih plinov, nevtronske difrakcije, spektri neelastičnega sipanja nevtronov).
- Študirali smo kemijsko reakcijo med končnim karcinogenom in polifenolom elagične kisline. Izračunali smo aktivacijsko prosto energijo z uporabo kvantno-kemijskih metod in različnimi metodami solvatacije. Dobro ujemanje

steroid dependent and related to the mechanism by which these molecules produce the anti-tumor activity. It is known, that small chemical modifications on the steroidal skeleton produce significant alternations on the anti-tumor activity.

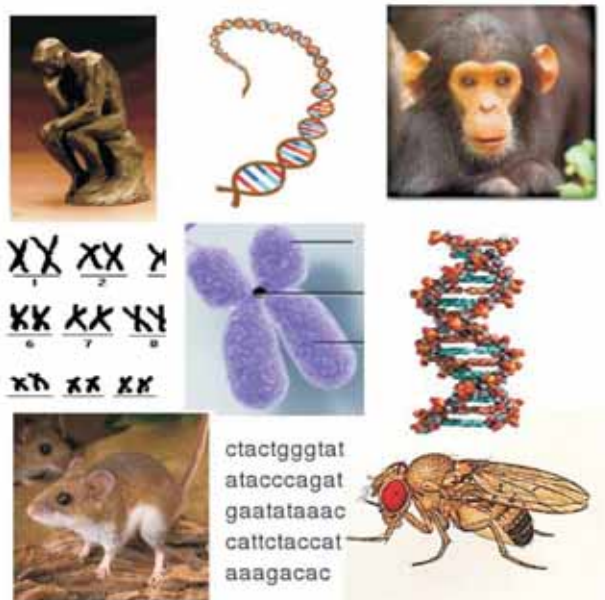
- Time dependent hydrogen-deuterium exchange in solid proteins was monitored by infrared spectroscopy. The exchange rate constants were calculated by applying difference spectroscopy, spectral decomposition and Laplace transformation. We have shown that the exchange rate constant depends on protein secondary structure and degree of solvent exposure. The analysis of the amide I band in the infrared spectrum of protein proves that the method suggested by coworkers extracts correctly folded protein. We also demonstrated that both ATR spectroscopy and calculated optical constants allow *in-situ* monitoring of chemical and electrochemical reactions. Using ATR spectroscopy and calculated absorbance spectra we explained the influence of hydrogen bonds on formation of hyper-branched polyester.
- Dynamics of hydrogen bonded protons with symmetrical or nearly symmetrical double-well potentials is strongly dependent on the environment. We have studied the dynamics of such systems using vibrational spectroscopy and molecular modeling. As model systems we used N-oxides of substituted picolinic acids because substituents strongly affect the strength of the hydrogen bond, which are also sensitive to environment. As model systems we used matrix isolated picolinic acid N-oxide. For this work experimental methods were used that are not available in Slovenia (infrared spectra in argon matrix, neutron diffractions, inelastic neutron scattering spectra).
- Chemical reaction between a polyphenol elagic acid and an ultimate carcinogen was studied. Activation free energy was calculated with medium high quantum-chemical

med eksperimentalno in izračunano bariero potrjuje pravilnost predpostavljenega mehanizma.

- Napravili smo vibracijsko analizo za OH način nihanja v substituiranih fenolih. Potencialno funkcijo smo dobili s kvantno kemijskimi metodami na visokem nivoju teorije. Vibracijsko Schroedingerjevo enačbo smo reševali numerično. Razlike med vibracijskimi nivoji se odlično ujemajo z eksperimentalnim vibracijskim spektrom.
- Z uporabo metodologije virtualnega reševanja in NMR spektroskopije smo potrdili vezavo 2-aminobenzimidazolnega in indolin-2-on-skega fragmenta na N-terminalni konec DNA giraze B, kar je omogočilo nadaljnjo optimizacijo inhibitorjev DNA giraze.
- Študirali smo mutabilnost poliadeninskih zaporedij v človeškem genomu. Pokazali smo, da je mutabilnost poliadeninov v področjih, ki so bogata z geni, nekoliko nižja, kot v predelih, kjer je gostota genov pod povprečjem.

methods in conjunction with various solvation models. Good agreement between the calculated and experimental activation free energy was found, confirming the validity of the proposed reaction mechanism.

- Vibrational analysis of the OH stretching vibration in substituted phenols was performed. Potential energy function was obtained by high level quantum calculations. The vibrational Schroedinger equation was solved and the differences between the eigenvalues were compared with the experimental vibrational spectrum. Good agreement between the theory and experimental values was found.
- Using the tools of virtual screening and NMR spectroscopy we identified the binding of 2-aminobenzimidazole and indolin-2-on fragments to the N-terminal fragment of DNA gyrase B what enabled further optimization of DNA inhibitors.



SLIKA 2:

Danes so poznana celotna genomska zaporedja številnih organizmov. Z njihovo primerjavo dobimo vpogled v evlucijske procese na molekularni ravni .

FIGURE 2:

Today several entire genomes are known. By comparing their sequences it is possible to get insight into the basic processes of molecular evolution.

- Pokazali smo tudi, da igrajo v mutacijskih procesih pomembno vlogo zaporedja kratkih razsejanih ponovitev, ki ne kodirajo neposredno proteinov ali strukturnih nukleinskih kislin, vplivajo pa na ekspresijo genov.
- V okviru dela na raziskovalnem programu P1-0002 smo v letu 2005 objavili 22 originalnih znanstvenih člankov, od tega 19 v SCI revijah, od katerih jih je 12 v SCI revijah iz prvega kvartila. Nekateri glavni dosežki so naslednji:
 - Razvili smo simplektično metodo SISM za simulacijo molekulske dinamike, ki omogoča šestkratno povečanje integracijskega koraka in s tem šestkratno pohitev simulacije molekulske dinamike tekoče vode v primerjavi s standardnimi metodami. Z našo metodo je mogoč izračun IR spektra vode, kjer ne pride do premika normalnih modov na račun hitrih vibracijskih nihanj vodikovih vezi.
 - Razvili smo vzporedne metode za vzporedno računanje simulacije molekulske dinamike s posebnim poudarkom na metodi SISM. To metodo smo priredili za vzporedno računanje na sistemih vzporednih računalniških gruč VRANA in MD-GRAPE procesorjih. Tako smo dosegli 8-krat hitrejše izvajanje simulacije molekulske dinamike v primerjavi s standardnimi vzporednimi računalniškimi gručami.
 - Razvili smo DFT pristope za izračun lastnosti elektronske strukture ogljikovih „armchair“ in „zig-zag“ nanocevk. Ugotovili smo, da so „armchair“ strukture manj reaktivne od „zig-zag“ struktur ter da so „armchair“ strukture električni prevodniki, medtem ko so „zig-zag“ strukture polprevodniki. Razvili smo tudi algoritme za obravnavo topoloških lastnosti periodičnih fullerenov.
 - S pomočjo QM-MM metod smo obravnavali stabilnosti kompleksov različnih konformer netropsina z DNA. Ugotovili smo pomembnost van der Waalsovih interakcij za določanje stabilnosti kompleksov netropsina in DNA.
 - S pomočjo ab-initio pristopov smo obravnavali Ugijeve multikomponentne reakcije in
 - Mutability of polyadenines was studied in human genome. It was shown that their mutability depends upon their location in chromosomes. Polyadenines which reside in the gene rich regions exhibit lower mutability than the ones residing in the regions where the gene density is below average. It was also shown that the short interspersed repeat elements which are not directly involved in coding of proteins or structural nucleic acids play an important role in polyadenine mutabilities and, consequently also in gene expression.
 - The results obtained in the framework of the research program P1-0002 were presented in the form of 22 original scientific articles, 19 of which were published in SCI journals and 12 of which are in the first quartile of SCI journals. Some of the major achievements are the following:
 - We have developed the SISM symplectic method for molecular dynamics simulations, which allows up to a six times longer integration time step and a corresponding six times faster molecular dynamics simulation of liquid water compared to standard methods. Our method enables the calculation of the IR spectrum of water in which no blueshifting of the stretching normal mode frequencies is observed as occurs with the standard method.
 - We have developed parallel methods for molecular dynamics simulation. An emphasis was placed on the SISM, which we parallelized to run on our VRANA clusters as well as multiple MD-GRAPE 2 processors, thus achieving up to a 8 fold speedup as compared to standard parallel computer clusters.
 - We have developed techniques based on the DFT for calculating the electronic structure of both armchair and zig-zag carbon nanotubes. We have determined that armchair nanotubes are less reactive than their zig-zag counterparts, as well as that armchair nanotubes are conductors while zig-zag nanotubes are semiconductors. We have also de-

ugotovili, da se anion in kation simultano vežeta na izocijanid ter da vmesna intermedijata nista stabilna.

- Utemeljili smo pomen zveze med obliko potencialnega polja, ki ga ustvarjajo molekule topljenca (biološke makromolekule) in ureditvijo molekul topila (vode). Vpeljali smo dva nasprotujoča si tipa parametrov reda za vodo, ki odražata princip maksimalne lokalne ureditve molekul vode (medsebojna orientacija molekul zaradi vodikovih vezi) in princip maksimalne globalne zgostitve. Pokazali smo, da je ureditev molekul vode ob površini proteinov povezana s prevlado enega izmed obeh principov, ki jo pogojuje oblika potencialnega polja proteina. Strukturo in dinamiko sistema smo simulirali s pomočjo molekulske dinamike. Razvili smo več splošnih metod in uporabnih računalniških programov (orodij) za analizo strukture in dinamike topila (vode) v neposredni bližini bioloških makromolekul.

veloped algorithms for studying the topological properties of periodic fullerenes.

- Using QM/MM methods we have studied the stabilities of complexes with different conformers of netropsin and DNA. We have determined the importance of van der Waals interactions to the stability of complexes with netropsin and DNA.
- By using the ab initio approach we have studied Ugi multicomponent reactions and determined that the anion and cation are bonded simultaneously to the isocyanide as well as that the intermediates are unstable.
- We have established the relation between the form of the effective potential field generated by the solute molecules (biological macromolecules) and the packing structure of the solvent molecules (water). We introduced two frustrated types of order parameters for water, which describe the principle of maximum local ordering of water molecules (ori-



SLIKA 3:

Dr. Dušanka Janežič, urednica revije *Journal of Chemical Information and Modeling*, je uredila posebno številko s 35 prispevki pretežno slovenskih avtorjev

FIGURE 3:

Dr. Dušanka Janežič, Associate Editor of the *Journal of Chemical Information and Modeling*, edited a special issue with 35 contributions of primarily Slovene authors

Izpeljane metodološke rešitve se odlikujejo po prikladnosti in po veliki računski učinkovitosti.

- D. Janežič je "Associate Editor" revije Journal of Chemical Information and Modeling (prej Journal of Chemical Information and Computer Sciences), An American Chemical Society Publication. Uredila je posebno številko JCIM-a, posvečeno Regionalnemu srečanju biofizikov, ki je bilo od 16. do 20. marca 2005 v Zrečah. V njej je objavljeno 35 člankov pretežno slovenskih avtorjev.
- M. Hodošček je soavtor in razvijalec najbolj uporabljanega računalniškega programa za molekularno modeliranje - CHARMM (Chemistry at HARvard Molecular Mechanics).

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Lek, d.d., Raziskave učinkovin, Ljubljana; raziskave novih učinkovin
- Institut Jožef Stefan, Ljubljana
- Medicinska fakulteta, Univerza v Ljubljani
- Fakulteta za matematiko in fiziko, Univerza v Ljubljani
- Biotehniška fakulteta, Univerza v Ljubljani
- Fakulteta za farmacijo, Univerza v Ljubljani
- Fakulteta za računalništvo in informatiko, Univerza v Ljubljani
- Univerza na Primorskem, Koper

MEDNARODNO SODELOVANJE

- Dr. Thomas Mavromoustakos, Institute of Organic and Pharmaceutical Chemistry, The National Hellenic Research Foundation, Athens, Grčija
- Prof. Aleksander Koll, Faculty of Chemistry, University of Wrocław, Poljska
- projekta NATO Collaborative Linkage Grant in COST D23, katerih odgovorni nosilec je M. Hodošček
- Bilateralni projekti (odgovorna nosilka: D. Janežič):

entational ordering due to hydrogen bonding), and the principle of maximum global density ordering. We have shown that the behaviour of the water molecules is driven by the prevailing of one of the two principles, which is modulated by the protein potential field. Structure and dynamics of the system were simulated by a molecular dynamics program. In order to analyze the structure and dynamics of solvent in the interfacial layer around biomolecules we have developed several methods and computer programs (tools) for the general use. These tools are distinguished by simplicity and computational efficiency.

- D. Janežič is an Associate Editor of the Journal of Chemical Information Modeling (formerly Journal of Chemical Information and Computer Sciences), An American Chemical Society Publication. She edited a special issue of JCIM dedicated to Regional Biophysics Meeting, held in Zreče, Slovenia, March 16. – 20. 2005 in which appeared 35 articles primarily of Slovene authors.
- M. 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

- Lek, d.d., Drug Discovery, Ljubljana, Slovenia: developing of novel chemical entities (NCE's)
- Jožef Stefan Institute, Ljubljana, Slovenia
- Faculty of Medicine, University of Ljubljana, Slovenia
- Faculty of mathematics and physics, University of Ljubljana, Slovenia
- Biotechnical Faculty, University of Ljubljana, Slovenia
- Faculty of Pharmacy, University of Ljubljana, Slovenia
- Faculty of Computer and Information Science, University of Ljubljana, Slovenia
- University of Primorska, Koper, Slovenia

z ZDA: dr. Bernard R. Brooks, National Institutes of Health, Bethesda, MD

s Hrvaško: dr. Sonja Nikolić, Institut Ruđer Bošković, Zagreb

s Hrvaško: dr. Sanja Tomić, Institut Ruđer 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, Budapest (medakademijski projekt)

POMEMBNI INŠTRUMENTI IN OPREMA

- NMR spektrometri v okviru Slovenskega NMR centra
- FTIR spektrometer Bruker IFS 66S
- PE 2000 NIR Ramanski spektrometer
- Računalniška oprema: SG delovne postaje, vzporedne računalniške gruče VRANA, sestavljene iz več kot 200 Athlon procesorjev

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Tomaž Mesar: Sinteza in biološka aktivnost tricikličnih karbapenemskih inhibitorjev beta-laktamaz, magistrsko delo; mentor: M. Kočevar, komentor: T. Šolmajer

INTERNATIONAL COLLABORATION

- Dr. Thomas Mavromoustakos, Institute of Organic and Pharmaceutical Chemistry, The National Hellenic Research Foundation, Athens, Greece
- Prof. Aleksander Koll, Faculty of Chemistry, University of Wroclaw, Poland
- We collaborate on the international NATO projects Collaborative Linkage Grant and COST D23 (M. Hodošček)
- Bilateral projects (principal investigator: D. Janežič) with researchers from the following countries:

USA: Dr. Bernard R. Brooks, National Institutes of Health, Bethesda, MD

Croatia: Dr. Sonja Nikolić, Institute Rudjer Bosković, Zagreb

Croatia: Dr. Sanja Tomić, Institute Rudjer Bosković, 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

MAJOR EQUIPMENT

- NMR spectrometers at Slovenian NMR Centre
- FTIR spectrometer Bruker IFS 66S
- PE 2000 NIR Raman spectrometer
- Computer hardware: SG workstations, parallel computer clusters VRANA, composed of more than 200 Athlon processors

EDUCATION AND IMPORTANT VISITS

- Tomaž Mesar: Synthesis and biological activity of tricyclic carbapeneme inhibitors of beta-lactamase (master degree thesis); mentor: M. Kočevar, comentor: T. Šolmajer

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. Lidija Slemenik Perše
Dr. Angela Šurca Vuk

**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Marko Bitenc
Mojca Fir
Robi Ješe
Vasko Jovanovski
Jelica Vince

TEHNIČNO OSEBJE / TECHNICAL STAFF

Miljana Horvatić
Helena Spreizer

PRIPRAVNIK / TRAINEE

Ivan Jerman



PODROČJA DEJAVNOSTI

Glavni poudarek je bil na razvoju komponent za energetske sisteme, ki izkoriščajo sončno sevanje: Grätzlove fotoelektrokemijske celice, barvne prevleke za absorberje sončnega sevanja, elektrokromna (pametna) optično preklonpa okna, fotokatalitska razgradnja okolju nevarnih snovi. Vzporedno je tekel razvoj analiznih in eksperimentalnih pristopov za raziskave strukture materialov, optičnih lastnosti (barva, termična emisivnost) in površinskih lastnosti (plazemske tehnologije in fotokataliza).

BIBLIOGRAFIJA

- 22 izvirnih znanstvenih člankov
- 1 strokovni članek
- 3 poljudni članki
- 1 samostojni znanstveni sestavek v monografiji
- 6 srednješolskih, osnovnošolskih ali drugih učbenikov z recenzijo
- 1 priročnik, slovar leksikon, atlas, zemljevid
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanje)

RESEARCH ACTIVITIES

In the year 2005 we continued with the development of materials, which are essential for the functioning of various devices and systems exploiting solar energy by converting it to either electricity or heat: dye-sensitized photoelectrochemical (DSPEC) cells of Grätzel type, electrochromic systems for controlling the solar radiation throughput in »smart« windows (passive devices) and solar absorbers for building facade collector systems. In parallel to these activities, we developed various methods for better understanding of the materials' properties such as their structure, optical properties (colour, thermal emittance), and their surface characteristics (for plasma deposition and photocatalysis).

BIBLIOGRAPHY

- 22 Original Scientific Articles
- 1 Professional Article
- 3 Popular Articles
- 1 Independent Scientific Component Part in a Monograph

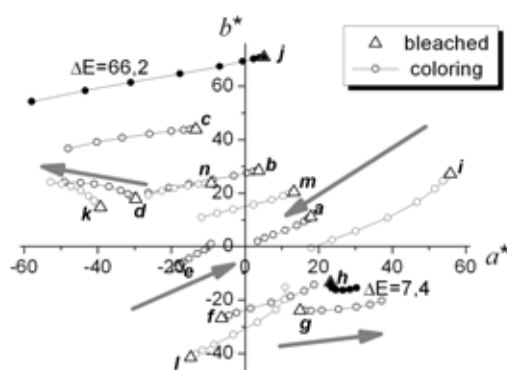
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| 9 objavljenih znanstvenih prispevkov na konferencah | 6 Reviewed Secondary and Primary School Textbook or other Textbook |
| 1 objavljeni strokovni prispevek na konferenci | 1 Manual, Dictionary, Lexicon, Atlas, Map |
| 29 objavljenih povzetkov znanstvenih prispevkov na konferencah | 1 Published Scientific Conference Contribution (Invited Lecture) |
| 4 objavljeni povzetki strokovnih prispevkov na konferencah | 9 Published Scientific Conference Contributions |
| 2 predavanji na tujih univerzah | 1 Published Professional Conference Contribution |
| 1 elaborat, predštudija, študija | 29 Published Scientific Conference Contribution Abstracts |
| 3 diplome | 4 Published Professional Conference Contribution Abstracts |
| | 2 Invited Lectures at Foreign Universities |
| | 1 Treatise, Preliminary Study, Study |
| | 3 Undergraduate Theses |

GLAVNI DOSEŽKI V LETU 2005

- S pomočjo surfaktantov smo pripravili nanokristalinične TiO₂ prevleke in prahove. Potrdili smo njihovo fotokatalitsko učinkovitost, s spektroskopskimi pristopi določili površinsko strukturo [A. Šurca Vuk et al., Int. J. Photoenergy 7, 163 (2005)] in interkalacijske lastnosti [A. Šurca Vuk et al., Sol. Energy Mater. Sol. Cells 90, 452 (2006)].
- Za elektrokromna preklonpa okna smo

IMPORTANT ACHIEVEMENTS IN 2005

- For DSPECs' cells TiO₂ films and powders were synthesized using different surfactants and their electrochemical properties were assessed and correlated with their surface struc-



SLIKA 1:

Sprememba standardiziranih barvnih vzorcev v prostoru z gasokromnimi preklonnimi okni med obarvanjem okna. Barvne spremembe so prikazane pri enaki svetlosti, to je v (a*,b*) ravnini enakozaznavnega CIELAB barvnega prostora. Največjo celokupno barvno razliko dobimo za intenzivno rumeni predmet ($\Delta E=66,2$), najmanjšo pa za svetlo rdeče-vijolični predmet ($\Delta E=7,4$). Puščice kažejo smeri barvnih sprememb.

FIGURE 1:

Color shifts of standardized color chips inside the room with gasochromic switchable windows during coloring. Color shifts are shown at equal lightness, i.e. on the (a*,b*) plane of the approximately uniform CIELAB color space. The largest total color change was obtained for strong yellow sample ($\Delta E=66,2$) and the smallest for the light reddish purple ($\Delta E=7,4$). Arrows indicate directions of color change due to coloration of the window.

nadaljavali s študijem protielektrod (V2O5 [A. Šurca Vuk et al., Chem. Anal. 50, 179 (2005)], Ce-V oksid [Z. Crnjak-Orel et al., Sol. Energy Mater. Sol. Cells 86, 19 (2005)]. Tako smo uspeli izboljšati lastnosti vanadijevega oksida s tem, da smo dodali pri sintezi organsko-anorganski hibrid (ormosil) [M. Liberatore, Sol. Energy Mater. Sol. Cells 90, 434 (2006)], z raziskavami Ce-V oksida pa smo potrdili njegovo uporabnost v praktičnih elektrokromnih sistemih. Študirali smo vpliv, ki ga ima zvezno spreminjanje prepustnosti elektrokromnega okna na videz predmetov. Barvne spremembe so izrazite in povzročijo nelinearne deformacije CIELAB barvnega prostora [M. Klanjšek Gunde, J. Opt. Soc. Am. A, Opt. Image. Sci. Vis. 22, 416 (2005)] (Slika 1).

- lonske tekočine so v zadnjem desetletju pritegnile interes javnosti zaradi svoje

ture, nanocrystallinity, surface area and vibrational spectra [A. Šurca Vuk et al., Int. J. Photoenergy 7, 163 (2005)]. Results confirmed their high photocatalytic activity expressed in the degradation ability of various compounds, photocatalytic splitting of water leading to superhydrophilic surfaces and capacity for electrochemical splitting of water, which was assessed from the large cathodic currents observed during the electrochemical charging/discharging of films in aprotic and protic electrolytes [A. Šurca Vuk et al., Sol. Energy Mater. Sol. Cells 90, 452 (2006)].

- For electrochromic applications we continued to develop counter electrodes having negligible cathodic colouration (V2O5 [A. Šurca Vuk et al., Chem. Anal. 50, 179 (2005)], Ce-V-oxide [Z. Crnjak-Orel et al. Sol. Energy Mater. Sol. Cells 86, 19 (2005)]). Certain im-



SLIKA 2:

Naslovna stran Kataloga premazov za Solabs EU projekt: uporaba spektralno selektivnega premaza ($a_s = 0.87$ and $e_r = 0.36$) na fasadi stavbe (Teufel-Schwartz, Avstrija).

FIGURE 2:

Initial page of the Catalogue of paint coatings for Slabs EU project: The application of Thickness Insensitive Spectrally Selective (TISS) paint coating ($a_s = 0.87$ and $e_r = 0.36$) on the facade of the building (Teufel-Schwartz, Austria).

zanemarljivo majhne hlapnosti in možnosti prevajanja različnih ionskih zvrsti. V primeru Grätzlovih celic predstavljajo alternativo običajnim ionskim elektrolitom z vključenimi redoks I^-/I_3^- pari. Za delo programske skupine pa predstavljajo nadgradnjo redoks elektrolitov, narejenih na osnovi organsko-anorganskih hibridov po postopkih sol-gel kemije, in to zato, ker zaradi njihove zanemarljive hlapnosti odpade potreba po tesnenju Grätzlovih celic. Ionske tekočine za Grätzlove celice so znane le 6 let in od takrat je bila narejena vrsta elektrolitov, ki so potrdili, da je raziskave v tej smeri vredno nadaljevati, nakazali pa so tudi, da predstavlja tesnenje celic še vedno problem. Od tod je le korak do uporabe ionskih tekočin, ki bi imeli kvazi trdno ali gelsko strukturo. Problem smo rešili tako, da smo sintetizirali ionsko tekočino (1-metil-3-[3-(trimetoksi- λ^4 -silyl)propil]imidazolijev jodid), ki je imela na imidazolijevem kationu pripete trietoksi skupine, ki so omogočile, da ionska tekočina kondenzira v kvazi trdno stanje [B. Orel et al., *Electrochem. Commun.* 7, 692 (2005); V. Jovanovski et al., *J. Phys. Chem. B* 109, 14387 (2005); B. Orel et al., *J. Nanosci. Nanotechol.* (v tisku)].

- Protonske prevodne membrane smo razvijali v okviru Apollon EU projekta (vodja S. Hočevar). Poizkusi na membranah v gorivnih celicah potekajo naprej, dodatne rezultate pa bomo objavili v letu 2006 [U. Lavrenčič Štangar, *J. Solid State Electrochem.* 9, 106 (2005)].
- Karbamatosilne nanokompozite smo uporabili v obliki gelov za pripravo redoks elektrolitov, ki omogočajo delovanje hibridnih elektrokromnih sklopov [V. Jovanovski, *Organosilicon Chemistry*, 2, 967 (2005)]. Prednost redoks elektrolitov je v tem, da ustrezni elektrokromni sistemi ne potrebujejo proti elektrod. Z vključevanjem ionske tekočine smo dosegli trajno elastičnost nanokompozita, do odhlapevanja reakcijskih produktov ni prišlo; k temu je pripomogla tudi

improvements were made for the V_2O_5 films with the addition of organic-inorganic hybrid to the initial sol of Vanadium isopropoxide precursor [M. Liberatore, *Sol. Energy Mater. Sol. Cells* 90, 434 (2006)]. The light vision of the interior of buildings equipped with "smart" windows colouring were quantified, revealing that the continuous variation of the light impinging through "smart" window led to the inversion of the colour space (Fig. 1). These types of study are not known and were published for the first time [M. Klanjšek Gunde, *J. Opt. Soc. Am. A, Opt. Image. Sci. Vis.* 22, 416 (2005)].

- Ionic liquids attracted interest worldwide in the last few years mainly because of their negligible vapour pressure, low toxicity and ability to conduct various ions, which open their applications as electrolytes for various electrochemical devices (batteries and DSPEC cells). We succeeded to prepare an ionic liquid showing self-condensation properties, avoiding the leakage problems encountered with the ordinary ionic liquids. The condensation of the ionic liquid was achieved by making 1-methyl-3-[3-(trimethoxy- λ^4 -silyl)propyl]imidazolium iodide, characterized by the trialkoxysilane groups enabling the sol-gel reactions, which led to the formation of positively charged silsesquixane condensation products having an open polyhedra structure (POSS) [B. Orel et al., *Electrochem. Commun.* 7, 692 (2005); V. Jovanovski et al., *J. Phys. Chem. B* 109, 14387 (2005); B. Orel et al., *J. Nanosci. Nanotechol.* (in press)].
- Proton conducting membranes were synthesized and applied in low-temperature fuel cells. This work was done in the frame of our collaboration in EU Project Apollon (S. Hočevar) [U. Lavrenčič Štangar, *J. Solid State Electrochem.* 9, 106 (2005)].
- The work published in [V. Jovanovski, *Organosilicon Chemistry*, 2, 967 (2005)] represents an alternative approach towards the preparation of electrochromic devices with a



SLIKA 3:

Meritve na IR spektrometru Bruker IFS 66/S.

FIGURE 3:

Measurements on an IR spectrometer Bruker IFS 66/S.

uporaba močnih kislin, katerih solvolizni produkti (t.j. estri) niso hlapni tako kot ustrezni alkoholi.

- Za študij sol-gel procesov (hidrolize, solvolize in kondenzacije) smo razvili pristope z infrardečo spektroskopijo ter uspeli pokazati, da sol-gel nanokompozitni hibridi na osnovi ureasilov tvorijo pri dodatku kislinjskih katalizatorjev aprotične gele, s čimer smo prispevali k rešitvi vprašanja, zakaj ureasili kažejo izrazito luminiscenco, če so kondenzirani z močnimi kislinami. Z infrardečo spektroskopijo smo tudi potrdili povezavo med strukturo gelov in tvorjenimi poliedričnimi silseskviokskanskimi strukturami z njihovo hidrofobnostjo [B. Orel et al., *J. Non-cryst. Solids* 351, 530 (2005); B. Orel et al., *J. Sol-Gel Sci. Technol.* 34, 251 (2005)]. Izsledke smo koristno uporabili pri ovrednotenju drugih nanostrukturnih hibridov [L. Armelao et al., *J. Mater. Chem.* 15, 1954 (2005)].
- Pripravili smo nizkoemisijske barvne premaze različnih nians (v okviru SOLABS EU projekta

hybrid structure. In this case carbatosil (diureasil) type organic-inorganic sol gel hybrid was used in the combination of ionic liquid used for DSPEC redox electrolytes.

- Some basic studies oriented in the understanding of the sol gel processes performed under hydrolysis and solvolysis (aprotic) conditions were done with the help of infrared and ^{29}Si NMR spectroscopic techniques. Results confirmed that under solvolysis conditions ureasil gels containing negligible amount of silanol groups and water formed. Such condition favours the luminiscence properties of ureasils and contributed to the high efficiency of the DSPEC cells employing sol gel redox electrolytes [B. Orel et al., *J. Non-Cryst. Solids* 351, 530 (2005); B. Orel et al., *J. Sol-Gel Sci. Technol.* 34, 251 (2005)].
- In the frame of SOLABS EU project and with the collaboration of Color factory (Medvode, Slovenia) various spectrally selective paints were prepared (Fig. 2). The corresponding paint coatings are characterized with strong

(Slika 2)) za fasadne sončne kolektorje ter ugotovili, da po svojih barvnih lastnostih in energetski učinkovitosti prekašajo analogne premaze, ki za doseganje energetske učinkovitosti izkoriščajo majhno debelino [Z. Crnjak Orel et al., Sol. Energy Mater. Sol. Cells 85. 41 (2005)] ter uporabili te izsledke za pripravo kamuflažnih premazov za termovizijsko zaščito objektov in naprav. Osnove za kvantifikacijo optičnih lastnosti učinkovitih premazov so bile izdelane na primeru praškastih premazov [M. Klanjšek Gunde et al., Prog. Org. Coat. 54, 113 (2005)] ter na plazemsko jedkanih plasteh [M. Klanjšek Gunde et al., Vacuum. 80, 189 (2005); M. Mozetič, Mater. Forum 29, 438 (2005)].

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Color d.d., Medvode; razvoj premazov za sončne zbiralnike in fasade (sodelovanje v okviru Solabs EU projekta in samostojnega projekta MORS)
- Helios d.d., Domžale, licenčna pogodba za izdelavo Solarect-Z premaza

MEDNARODNO SODELOVANJE

- *In-situ* spektroskopske analize elektrooptičnih sistemov, ogledal, fotonapetostnih celic in prikazalnikov, Proteous - bilateralno sodelovanje Slovenija - Francija, 2004 – 2005; P. Colomban, CNRS, LADIR, Thiais-Pariz, Francija (B. Orel)
- Nanoporozni sol-gel materiali za elektrokromne aplikacije, bilateralno sodelovanje Slovenija - Italija 2002 – 2005; F. Decker, Università "La Sapienza", Rim, Italija (A. Šurca Vuk)
- Development of unglazed solar absorbers (resorting to coloured selective coatings on steel material) for building facades and integration into heating systems (SOLABS), RTD projekt, 2003 - 2006 (B. Orel)
- Polymeric Materials for Solar Thermal Applications, International Energy Agency (IAE),

colours (metric chroma $C^* > 13$) and spectral selectivity (a_{λ}/e_{λ}) which imparted them performance higher compared to those of black spectrally non-selective paint coatings. The photothermal conversion properties of the paints did not depend on the coating thickness and they exhibited stronger colours compared to the analogues paints, the spectral selectivity of which depends on their thickness [Z. Crnjak-Orel et al., Sol. Energy Mater. Sol. Cells 85. 41 (2005)]. Basics of the quantification of optical properties of effect coatings were studied on powder coatings [M. Klanjšek Gunde et al., Prog. Org. Coat. 54, 113 (2005)] and plasma etched layers [M. Klanjšek Gunde et al., Vacuum. 80, 189 (2005); M. Mozetič, Mater. Forum 29, 438 (2005)].

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Color d.d., Medvode, Slovenia; development of spectrally selective coatings for solar collectors and facades (cooperation in the frame of Solabs EU project and project from MORS)
- Helios d.d., Domžale, Slovenia; licence contract for production of the Solarect-Z paint

INTERNATIONAL COLLABORATION

- *In-situ* spectroscopic analysis of electrooptic systems, mirrors, photoelectrochemical cells and displays, Proteous - bilateral cooperation Slovenia - France 2004 - 2005, P. Colomban, CNRS, LADIR, Thiais-Paris, France (B. Orel)
- Nanoporous sol-gel materials for electrochromic application, bilateral cooperation Slovenia - Italy 2002 - 2005, F. Decker, University of Rome "La Sapienza", Rome, Italy (A. Šurca Vuk)
- Development of unglazed solar absorbers (resorting to coloured selective coatings on steel material) for building facades and integration into heating systems (SOLABS), RTD project 2003 - 2006 (B. Orel)
- Polymeric Materials for Solar Thermal Appli-

- sprejet projekt (december 2005); prošnja za pridruženo sodelovanje
- Mreža odličnosti: Nanostructured and Functional Polymer-based materials and Nanocomposites; Proposal No. NOE 500361-2 (Z. Crnjak Orel)
 - Raziskave neurejenih materialov: nano optični nanosi; bilateralno sodelovanje Slovenija - Hrvaška 2004 - 2006, Institut Ruđer Bošković, Zagreb, Hrvaška (Z. Crnjak Orel)
 - Priprava in karakterizacija uniformnih delcev, bilateralno sodelovanje Slovenija - ZDA, 2004 - 2005, Clarkson University, Potsdam, New York, ZDA (Z. Crnjak Orel)
 - Commission internationale de l'éclairage (CIE), Division 1 (M. Klanjšek Gunde, uradna članica)
 - CIE, Division 2, TC2-53 Multi-geometry color measurements of effect materials (M. Klanjšek Gunde, članica)
 - CIE, Division 1, TC1-66 Indoor daylight illuminant (M. Klanjšek Gunde, članica)

POMEMBNI INSTRUMENTI 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 potenciostat/galvanostat

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Robi Ješe, Jelica Vince, Mojca Fir, Vasko Jovanovski (mladi raziskovalci, mentor: B. Orel)
- Aljaž Vilčnik in Boštjan Japelj (komentor: B. Orel)
- Daša Šivec (praktikantka, mentor: B. Orel)
- Jure Ahtik (komentor: M. Klanjšek Gunde)
- Andraž Kocjan (diplomsko delo, delovni mentor: Z. Crnjak Orel)
- Katarina Demšar (diplomsko delo, delovni mentor: Z. Crnjak Orel)

cations, International Energy Agency (IAE), accepted project (December 2005), application for an associated cooperation

- Network of excellency: Nanostructured and Functional Polymer-based materials and Nanocomposites, Proposal No. NOE 500361-2 (Z. Crnjak Orel)
- Investigation of disordered materials: nano optic coatings, bilateral cooperation Slovenia - Croatia 2004 - 2006, Rudjer Boskovic Institute, Zagreb, Croatia (Z. Crnjak Orel)
- Preparation and characterisation of uniform particles, bilateral cooperation Slovenia - USA 2004 - 2005, Clarkson University, Potsdam, New York, USA (Z. Crnjak Orel)
- Commission internationale de l'éclairage (CIE), Division 1 (M. Klanjšek Gunde)
- CIE, Division 2, TC2-53 Multi-geometry color measurements of effect materials (M. Klanjšek Gunde)
- CIE, Division 1, TC1-66 Indoor daylight illuminant (M. Klanjšek Gunde)

MAJOR EQUIPMENT

- FT-IR spectrometer Bruker IFS 66/S
- FT-IR and FT-Raman spectrometer Perkin Elmer 2000
- Hewlett-Packard 8453 diode array UV-VIS spectrophotometer
- AUTOLAB PGSTAT30 and EG&G PAR 273 potentiostat/galvanostat

EDUCATION AND IMPORTANT VISITS

- Robi Ješe, Jelica Vince, Mojca Fir, Vasko Jovanovski (young researchers, mentor: B. Orel)
- Aljaž Vilčnik and Boštjan Japelj (comentor: B. Orel)
- Daša Šivec (practical work, mentor: B. Orel)
- Jure Ahtik (comentor: M. Klanjšek Gunde)
- Andraž Kocjan (degree, working mentor: Z. Crnjak Orel)
- Katarina Demšar (degree, working mentor: Z. Crnjak Orel)

L03

Laboratorij za kemometrijo

Laboratory of Chemometrics



VODJA / HEAD
Dr. Marjana Novič

RAZISKOVALCI / RESEARCHERS

Dr. Marjan Vračko
Dr. Neva Grošelj
Dr. Marjan Tušar (od / since 1. 12. 2005)
Dr. Milan Randić (3 mesece na leto / 3 months per year)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Špela Župerl
Viktor Drgan

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

Elena Boriani (6 mesecev / 6 months)
Morena Spreafico (2 meseca / 2 months)
Anna Karawajczyk (3 mesece / 3 months)

RAZISKOVALEC NA PO-DOKTORSKEM DELU IZ TUJINE / YOUNG POST-DOC SCIENTIST FROM ABROAD

Dr. Sylwester Mazurek (11 mesecev / 11 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 strukturalni kemiji, v QSAR študijah, v proteomiki in genomiki
- Študij algoritmov in razvoj programskih paketov
- Uporaba kemometričnih metod v analizi kemiji: zagotavljanje in kontrola kvalitete (QA/QC)
- Raziskave 3D reprezentacij kemijske strukture za uporabo v QSAR

RESEARCH ACTIVITIES

- Introduction of chemometrics, i.e., mathematical, statistical and computational methods for solving chemical problems, into 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 na področju kemometrije: v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani na diplomskem in podiplomskem nivoju
- 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
- 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 EU projects within Marie Curie training networks

BIBLIOGRAFIJA

- 18 izvirnih znanstvenih člankov
 - 1 strokovni članek
 - 2 samostojna znanstvena sestavka v monografiji
 - 3 intervjuji
 - 1 drugi članek ali sestavek
 - 3 objavljeni znanstveni prispevki na konferencah
- 22 objavljenih povzetkov znanstvenih prispevkov na konferencah
 - 1 objavljeni povzetek strokovnega prispevka na konferenci
 - 2 vabljeni predavanji na konferencah brez natisa
 - 1 diploma
 - 4 uredništva revij

DOSEŽKI V LETU 2005

- Raziskovalno delo Laboratorija za kemometrijo za leto 2005 je prikazano v 18 znanstvenih člankih in dveh poglavjih v monografijah, o rezultatih smo poročali v 22 prispevkih na mednarodnih in 3 prispevkih na domači znanstveni konferenci. V letu 2005 smo nadaljevali delo na programu *Modeliranje relacij med kemijsko strukturo in lastnostjo snovi - QSAR – QSPR*. Na področju, kjer program združuje kemometrijske raziskave L03 z analiznimi iz Zavoda za zdravstveno varstvo Maribor (ZZVMB), smo uspeli vzpostaviti dobro sodelovanje, katerega rezultati se kažejo med drugim v

BIBLIOGRAPHY

- 18 Original Scientific Articles
 - 1 Professional Article
 - 2 Independent Scientific Component Parts in Monographs
 - 3 Interviews
 - 1 Other Article or Component Part
 - 3 Published Scientific Conference Contributions
- 22 Published Scientific Conference Contribution Abstracts
 - 1 Published Professional Conference Contribution Abstract
 - 2 Unpublished Invited Conference Lectures
 - 1 Undergraduate Thesis
 - 4 Journal Editorships

ACHIEVEMENTS IN 2005

- The research work of the Laboratory of Chemometrics in 2005 is demonstrated in 18 scientific papers and two chapters in the monograph, the results were reported in 22 contributions at international and 3 at national scientific conferences. In 2005 we continued the work on the research program "Modelling of structure–property relationships – QSAR–QSPR". In the field, where the chemometrics research work of the Laboratory of Chemometrics is combined with the analysis made by the Institute of Public Health

kompleksni kemometrijski obravnavi analiznih rezultatov vodnih vzorcev (monitoringa vodnjakov, površinskih voda itd.) in hrane (jedilnega olja). Poudariti želimo, da so v ZZVMB na vzpodbudo, osnovano v okviru naše programske skupine, začeli že sredi leta 2005 spremljati prisotnost določenih pesticidov (metolaklor in njegovih razgradnih produktov) v površinskih vodah. Metolachlor je poznan kot selektivni herbicid, ki ga uporabljajo za zatiranje določenih vrst trave in širokolistnega plevela. Je zelo polarna spojina, zato se hitro izpere s površine v podzemne vode. To je izjemno pomemben projekt, saj je v ZDA metolaklor zaradi njegovih škodljivih lastnosti v okolju že prepovedan, medtem ko se v Evropi taka direktiva še pripravlja.

- Na področju QSAR raziskav smo proti koncu leta 2005 zaključili evropski projekt z naslovom "Kemometrijska obdelava spojin, ki motijo delovanje žlez z notranjim izločanjem". V času trajanja projekta je prišlo k nam na dodoktorsko izpopolnjevanje šest študentov iz različnih evropskih držav za skupno dobo 32 mesecev. Samo v letu 2005 smo gostili dve študentki iz Italije in eno iz Nizozemske.
- Leta 2005 smo začeli aktivno izvajati raziskave na evropskem projektu IBAAC, in sicer s kemo-informacijskim prispevkom na področju iskanja in optimizacije katalizatorjev za asimetrično kemijsko sintezo. Ta projekt poteka v okviru Marie Curie izobraževalne mreže, v kateri so sredstva namenjena za plačilo dela do- in podoktorskih študentov iz tujine. Od 1. februarja 2005 je v tem projektu vključen poljski podoktorski študent, ki je bil prve tri mesece na treningu pri švicarskem partnerju IBAAC projekta, profesorju Thomasu Wardu iz Univerze v Neuchatelu, Švica, potem pa je delo nadaljeval v našem laboratoriju.
- V letu 2005 smo začeli tudi delo na evropskem projektu TRACE, ki obravnava sledljivost

Maribor (IPHMB), we succeeded to establish good collaboration. The results are shown in several complex chemometrics analyses of the data, i.e. water samples obtained from monitoring of water wells, surface waters etc., and food samples (oil). We would like to stress that, on the initiative from our program group, the IPHMB started in the middle of the year 2005 with monitoring of certain pesticides (metolachlor and degradation products) in surface waters. Metolachlor is known as a selective herbicide used to control specific annual grasses and broadleaf weed. It is highly polar and thus leachable into the groundwater. This is a very important project, because the use of metolachlor in USA is already prohibited for its adverse effects on environment and wildlife, while in Europe similar directives are being prepared.

- In the QSAR field we finished the EU project of "Chemometrical treatment of endocrine disrupters". In the whole financing period of this project, we hosted six doctoral students from several European countries, altogether for 34 months. Only in 2005 there were two students from Italy and one from the Netherlands.
- In 2005 we have started with the activities in European project IBAAC. Our task is a chemoinformatics research in the field of catalysts design and optimization of reactivity parameters for asymmetric chemical synthesis. This project runs in the frame of Marie Curie Training Networks in which the funding is available for graduate and postgraduate students from abroad. On February 1st 2005 a Polish young researcher joined us as a post-doctoral fellow of IBAAC project. He spent first three months on training in the laboratory of a Swiss partner of IBAAC project, professor Thomas Ward from University of Neuchatel, Switzerland. Now he is doing his research work at our Laboratory.
- In the year 2005 we started also with new EU project, TRACE, which is about the trace-

hrane. Udeleženi smo v 6. delovnem paketu, ki je zadolžen za statistično obravnavo analiznih rezultatov zemlje, vode in določenih produktov (npr. olja, mesa, medu). Naša naloga je razviti orodje na osnovi umetnih nevronske mreže v MATLAB okolju. Delne rezultate smo prikazali na sestankih TRACE projekta.

- Kot je razvidno iz bibliografije, smo bili aktivni na področju kemometrijskih metod in aplikacij, kot sta npr. klasifikacija, karakterizacija vzorcev, na področju QSAR študij in na področju teorije grafov z uporabo v strukturnih reprezentacijah, v proteomiki in genomiki. Od 1. marca 2005 do 31. decembra 2005 je bil sodelavec L03 (M. Vračko) gostujoč znanstvenik (Senior Scientist Visitor) v Združenem raziskovalnem centru (European Chemical Bureau, Institute for Health and Consumer Protection, Joint Research Centre, Ispra, Italija). Tam je imel možnost predstaviti najrazličnejše računske (modelne) metode, ki bi jih eventualno lahko v bodoče uporabljali kot pomoč pri ocenjevanju kemikalij znotraj evropske regulatorne politike. S tem je razširil in utrdil pomen raziskovalnega dela L03, ki lahko ponudi kemometrijska orodja, ki so plod dolgoletnega razvoja algoritmov in kemometrijskih metod v laboratoriju.
- Za podjetje Lek Pharmaceuticals, d.d., Ljubljana smo uspešno zaključili industrijski projekt, ki smo ga izvajali kot eden od partnerjev in rezultati kažejo na možnost nadaljevanja in razširitve naloge. Naš prispevek je kemometrijsko ovrednotenje podobnosti / identičnosti kemijskih struktur nekaterih učinkovin.
- V letu 2005 smo dokončno postali solastniki mednarodnega podjetja VICIM BV s sedežem na Nizozemskem. Podjetje je bilo ustanovljeno v nadaljevanju Evropskega projekta VICIM iz evropskega 5. okvirnega programa, katerega partner je bila tudi naša skupina za kemometrijo. Podjetje bo opravljalo kemometrijske in metrološke usluge za naročnike, ability and origin of food. The project is financed within the Sixth European Framework programme as an Integrated project, Priority 5, Food Quality and Safety. Our Laboratory is included as a partner of Workpackage 6 (WP6), responsible for statistical specifications of analytical data of the soil, water, and food products (oil, meat, and honey). The funding is available for the research work with the aim to develop a toolbox for Artificial Neural Network in MATLAB environment. Partial results were already shown on the WP6 team meetings.
- Our activity was dedicated to application of chemometrical methods in different fields. In QSAR we applied methods for classification and characterisation of molecules. We applied the graph theory to represent molecular structures, the proteomic data and the genomic data. More details about the activities can be found in the reference list. One of the members (M. Vračko) has been appointed as Senior Visiting Scientist at the European Chemical Bureau, Institute for Health and Consumer Protection, Joint Research Centre, Ispra, Italy for the period from March 1 to December 31, 2005. He had the opportunity to present different computational (chemometrical) tools and models, which can be eventually used for assessment of chemicals in the framework of REACH legislation. It can be regarded as a recognition for the L03, which research has been oriented over the last years to development and promotion of chemometrical technics and tools.
- Industrial project with Lek Pharmaceuticals d.d., Ljubljana, Slovenia, in which we have been involved as one of the partners, was successfully finished and the results are showing a possibility of continuation and extension of the project. Our contribution is a chemometrics evaluation of similarity / identity of chemical structures of certain drugs.
- In 2005 we finally became shareholders of international company VICIM B.V. with the

kot je bilo predvideno že v času trajanja projekta.

- Pod mentorstvom naših sodelavcev in v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani je bilo v letu 2005 končano diplomsko delo Viktorja Drgana, *Matematični opis separacijskih procesov na anionski hidroksid-selektivni stacionarni fazi*. Viktor Drgan se je po diplomi vključil v skupino L03 kot mladi raziskovalec in bo delal na področju teoretičnega in eksperimentalnega raziskovanja ionske kromatografije, tako izokratske kot gradientne tehnike.

KRATEK OPIS DELA IN REZULTATOV

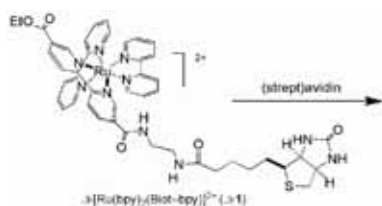
Na področju QSAR raziskav smo nadaljevali delo na motilcih žlez z notranjim izločanjem, začeli študijo o mehanizmu prenosa nekaterih antioksidantov preko celične membrane z bilitranslokazo, ter razširili uporabo grafično-teoretičnih invariant v proteomiki in genomiki. Projekt "Kemometrijska obdelava motilcev žlez z notranjim izločanjem" smo zaključili proti koncu leta 2005 s skupnim delom treh doktorskih študentk iz tujine (Italije in Nizozemske). Zgradili smo modele na osnovi protitočne nevronske mreže, ki zmorejo napovedovati vezavne konstante različnih spojin na estrogen receptor (ER) alfa in beta.

headquarter in the Netherlands. The company was established as a spin-off of a EU project financed in the 5th Framework Programme; our Laboratory was one of the partners in this project. The company will promote, as established already in the UE project, cost-effective chemical measurement practices by making use of modern chemometric approaches and develops procedures for adequate assessment of the quality of methods and measurement results.

- One diploma work was finished in 2005 under the mentorship of our co-workers and in collaboration with Faculty of Chemistry and Chemical Technology of the University of Ljubljana, Slovenia. The diploma thesis of Viktor Drgan was "Mathematical description of separation processes on anion hydroxide-selective stationary phase". Viktor Drgan joined our Laboratory as a young researcher and will work in the field of theoretical and experimental research of ion chromatography, in isocratic as well as gradient technique.

SHORT DESCRIPTION OF RESEARCH AND RESULTS

In QSAR research area we continued with the endocrine disrupters studies, we began to study the role of a membrane transmitter bilitranslocase in bioavailability of some anti-oxi-



SLIKA:

Streptavidin kot gostitelj za koordinacijske komplekse, vezane na biotin (Δ -[Ru(bpy)₂(Biot-bpy)]²⁺ (Δ -1)). Levo: biotiniziran koordinacijski kompleks. Desno: dva kompleksa ugnezdena v dimero streptavidina.

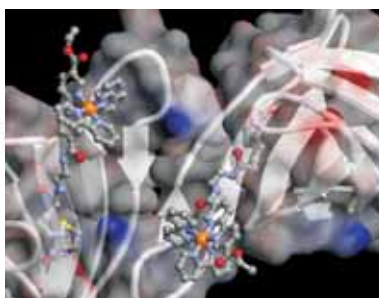


FIGURE:

Streptavidin as host for biotinylated coordination complex (Δ -[Ru(bpy)₂(Biot-bpy)]²⁺ (Δ -1)). Left: biotinylated coordination complex. Right: two complexes docked into a streptavidin dimere.

Določene spojine, kot so estrogene kemikalije, fitoestrogeni, naravni in sintetični estrogeni, so bili obravnavani z različnimi metodami: s pristopom, ki temelji na iskanju konformacije liganda z najmanjšo energijo in na podlagi te konformacije izračuna deskriptorje, ter s pristopom, osnovanim na strukturi, ki upošteva tudi strukturo proteina in za izračun deskriptorjev uporabi konformacijo, ki je rezultat metode ugnezdenja (docking). Z namenom dobiti najboljši možni model smo za izbor spremenljivk uporabili genetski algoritem (GA). Končni modeli, dobljeni za ER alfa in beta, so bili testirani z zunanjim testnim nizom.

Velik del raziskav smo posvetili razvoju in uporabi topoloških indeksov. Vzpostavili smo široko sodelovanje z mnogimi strokovnjaki s področja teorije grafov. Plod tega sodelovanja je razviden iz bibliografije; teoretične invariante, pridobljene s pomočjo teorije grafov, smo uspešno uporabili v proteomiki in genomiki. Za reševanje zgoraj omenjene industrijske naloge smo uporabili znanje in algoritme, ki so izhajali iz graf-teoretičnih raziskav.

V okviru evropskega projekta TRACE (Food Quality and Safety) smo obravnavali podatke, ki so dobljeni z analizo zemlje na površju in analizo sloja zemlje neposredno pod površjem, na treh različnih mestih jemanja vzorcev, s tremi različnimi sestavami zemlje (peščenjak, apnec, skrilavec). Skupno podatkovna baza zajema 180 vzorcev za vrhno plast ter 45 vzorcev za sloj zemlje neposredno pod površjem, vzorčevanih z devetih odvzemnih mest. Do sedaj opravljeno delo se nanaša na pripravo normaliziranih podatkovnih setov in vnos ključa za manjkajoče podatke. Določili smo tudi oznake glede na različne parametre, ki jih želimo slediti: ali odvzemna mesta glede na vrsto kamnine, ali glede na geografsko področje ali glede na koncentracijo elementov v zemlji. Tako pripravljene podatke smo s pomočjo Kohonenovih nevronskih mrež mapirali in klasificirali. V sklopu TRACE projekta se je ena sodelavka aprila 2005 udeležila prvega letnega sestanka v Yorku v Veliki Britaniji. Sestanek je potekal na temo

dants, and we expanded the applications of graph-theoretical invariants in proteomics and genomics. The project "Chemometrical treatment of endocrine disrupters" was completed in 2005 by a joint comparative work of three doctoral fellows. The CPNNs (Counterpropagation Neural Networks) models for prediction of experimental binding affinity of a range of substances towards estrogen receptor alpha and beta. Several compounds as estrogenic chemicals, phytoestrogens and natural and synthetic estrogens were treated with different methods: ligand-based approach, that finds out the minimum energy conformation as the most suitable conformation on which descriptors are calculated, and structure-based approach, that involves the use of protein structure, and uses conformations that are output of a docking methodology to calculate descriptors. Models were built up through training the counter-propagation neural network and encoding the information present in the two sets of molecular descriptors. In order to reach the best possible model, a selection of the descriptors using Genetic Algorithm (GA) was performed for both approaches. The final models obtained for estrogen receptor alpha and beta were tested with an external test set.

A large part of the research was directed into the development and application of topological indices. We established a broad collaboration with many experts from the graph-theoretical research area. The achievements can be seen from the reference list; graph-theoretical invariants have been successfully applied to proteomics and genomics. It has to be stressed here, that the knowledge and algorithms, emerging from graph-theoretical studies, were the basis for solving a part of the industrial project mentioned above.

In the frame of TRACE project (Food Quality and Safety) the first available dataset has been processed. Three teams were involved in sampling and analysis of soil data. 20 topsoil samples were randomly collected on three sample sites, all within 3 different lithologies (sand-

Sledljivost in izvor hrane (Traceability and the origin of food). Opisano delo je bilo septembra 2005 predstavljeno na sestanku skupine v Bruslju v Belgiji.

Na področju ocenjevanja kemikalij smo skupaj z Zavodom za zdravstveno varstvo Maribor sprožili pobudo za spremljanje določenih pesticidov v vodi. V L03 smo naredili temeljit literaturni pregled, medtem ko so v ZZVMB sredi leta 2005 začeli z meritvami. Za boljše poznavanje vplivov biocidov in herbicidov na zdravje ljudi se je sodelavka udeležila bazičnega izobraževanja, ki poteka v okviru slovensko - nizozemskega bilateralnega projekta "Risk assessment of chemicals with focus on biocides", ki je bil sklenjen med Uradom Republike Slovenije za kemikalije in Royal Haskoning, Nizozemska. Obdelane so bile naslednje tematike: Ocenjevanje izpostavljenosti za poklicne in nepoklicne uporabnike biocidov (november 2004), Toksikologija (januar 2005), Ekotoksikologija (februar 2005), ter Izpostavljenost za delavca in uporabnika ter ocena tveganja (junij 2005).

Sodelavcec, ki je bil od 1. marca do 31. decembra 2005 gostujoči znanstvenik v evropskem Združenem raziskovalnem centru (Senior Scientist Visitor in European Chemical Bureau, Institute for Health and Consumer Protection, Joint Research Centre, Ispra, Italija), nam je omogočil sodelovanje v diskusijah na ravni evropske regulatorne politike za področje ocenjevanja kemikalij. Na evropskem trgu je približno 100.000 registriranih kemikalij. Fizikalno - kemijski, toksikološki in ekotoksikološki podatki, skratka podatki, ki omogočajo oceno tveganja, so znani le za majhen del teh kemikalij. Kot temelj skupne kemijske politike Evropska Komisija predlaga REACH, to je transparenten sistem za registracijo, evaluacijo in avtorizacijo kemikalij. REACH zahteva zbiranje in sistematsko urejanje podatkov za obstoječe in nove kemikalije. Pred izvajalce so postavljene tri glavne naloge: (i) določitev prioriteta za testiranje za obstoječe kemikalije, (ii) klasifikacija in označevanje

stone, limestone, shale). In total, there were 9 sample sites and 180 sampling locations (for top-soil). In addition to the topsoil samples, the subsoil samples at 9 randomly chosen sampling locations within each site were obtained from locations lower below the surface. In total, there were 45 subsoil-sampling locations. Pre-processing of data included the normalization of the data sets and the incorporation of the key for missing data. The sample labels were also determined, following different parameters such as sampling sites regarding lithology or geographic area, and concentrations of the elements in the soil. So pre-processed data were mapped and classified with the application of Kohonen neural networks. The work was presented on the 3rd WP6 meeting in September 2005 in Brussels, Belgium. In the frame of this project one of the member of our laboratory attended the first annual meeting in April 2005 in York, U.K. The meeting was the official launch of TRACE with the main subject "Traceability and the origin of food".

Regarding assessment of chemicals, we initiated together with the the Institute of Public Health Maribor, Slovenia the initiative for the monitoring of certain pesticides in water. The literature search was accomplished in L03, while the IPHMB started with chemical analyses. On the ground of better knowledge about the influence of herbicides and biocides on the human health, our co-worker attended the training in the frame of Slovenian - Netherlands bilateral project entitled "Risk assessment of chemicals with focus on biocides". This is the project between the National Chemicals Bureau, Slovenia, and the Royal Haskoning, Netherlands. The topics of the training were: General aspects of exposure assessment (November 2004), Toxicology (January 2005), Ecotoxicology (February 2005), and Exposure estimation for the worker and the user along with the risk assessment (June 2005).

One of the members (M. Vračko) has been appointed as Senior Visiting Scientist at the European Chemical Bureau, Institute for Health and

kemikalij, (iii) ocean tveganja za obstoječe in nove kemikalije.

REACH, kot tudi širša mednarodna skupnost (OECD, "Organization for Economic Cooperation and Development") podpirata uporabo računalniških metod, vključno s (Q)SAR modeliranjem pri omenjenih nalogah. Ker so številni računalniški modeli že v uporabi, je OECD prevzela pet principov za oceno in validacijo (Q)SAR modelov, ki se uporabljajo v regulacijske namene.

V okviru projekta v JRC, Ispra, Italija, ki ga vodi sodelavec L03, smo postavili model za toksičnost za ribe (*Pimephales Promelas*). Uporabili smo metodo nevronske mreže, ki smo jo prilagodili za modeliranje in klasifikacijo spojin glede na vodno toksičnost. Sestavili smo obširno poročilo, v katerem smo predstavili nevronske mreže v luči OECD principov. Da bi dosegli kar najširše soglasje, smo na ECB organizirali srečanje 17 ekspertov iz področja kemometrije, kemijske regulative in industrije. Srečanje je bilo od 7. do 8. julija 2005 v JRC, Ispra, Italija, vodil ga je M. Vračko. Podrobnosti in sklepi bodo objavljeni kot recenziran znanstveni članek. Deli tega poročila so bili dodani k dokumentu, ki ga JRC pripravlja za OECD in katerega osnutek je bil predstavljen na srečanju OECD partnerjev 1. decembra 2005 v Parizu, Francija.

Na koncu naj predstavimo še naš doprinos k IBAAC projektu, in sicer gre za kemo-informacijski pristop k oblikovanju in optimizaciji katalizatorjev za stereospecifično hidrogenacijo. Vključili smo se v raziskovalno delo profesorja Thomasa Warda, ki je s pomočjo vgrajevanja kovinskega katalizatorja v proteinsko okolje zelo izboljšal stereo-specifičnost katalizatorja (ee%). Kovinski katalizator preko različnih vmesnih delov molekul (vmasnikov) pripnejo na biotin, ta pa ima zelo močno afiniteto do avidina ali streptavidina. Naša naloga je s pomočjo računalniškega paketa "Autodock" najti pozicijo (3D atomske koordinate) vsakega pripravljenega katalizatorja v proteinskem vezavnem žepu. Ker pa nastopa protein kot dublet dubleta, je naloga dokaj zahtevna. V nadaljevanju imamo namen

Consumer Protection, Joint Research Centre, Ispra, Italy for the period from March 1 to December 31, 2005. We can participate in the discussion of European chemical regulatory policy. European Chemical Bureau put one of our data sets (data set of endocrine disrupters) on its webpage (<http://ecb.jrc.it/QSAR/>). On the European market are about 100.000 registered chemicals and only for a part of them the data necessary for risk assessment are known (physico-chemical, toxicological, and ecotoxicological data). As a basis for common chemical policy the Commission has been proposing the REACH – a transparent system for Registration, Evaluation and Authorisation of Chemicals. REACH requires systematic maintaining of database for existing and new chemicals. The research priorities are: (i) the priority setting for existing and new chemicals, (ii) the classification and labelling of chemicals, (iii) the risk assessment of existing and new chemicals.

REACH and the broader society (OECD, Organization for Economic Cooperation and Development) support the using of computational methods including (Q)SAR models in mentioned tasks. Due to the fact that many regulatory agencies already have been using the (Q)SAR methods the OECD adopted five principles for validation of (Q)SAR models used for regulatory purposes.

In the framework of project in JRC in Ispra we proposed a model for aquatic toxicity for fish *Pimephales Promelas*. As a modeling technique we applied counter propagation neural network, which was adopted for modeling and classification accordingly the aquatic toxicity. In the report we presented the mentioned neural network technique in the light of OECD principles. For discussion and to reach the broad consensus the ECB organized the meeting of 17 experts from research institutions, regulatory agencies and industry. The meeting was held from July 7-8, 2005 in JRC, Ispra, Italy and was chaired from M. Vračko. The details and conclusions will be published in the peer reviewed journal. A part of this report has been

s pomočjo strukturnih deskriptorjev kompleksa metal-ligand-protein cele serije katalizatorjev optimizirati tako strukturo vmesnikov kot tudi morebitnih mutacij na proteinu, tako da bi izboljšali ee% kemijske reakcije.

SODELOVANJE Z INDUSTRIJO

- Lek Pharmaceuticals, d.d., Ljubljana

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

MEDNARODNO SODELOVANJE

mednarodni projekti:

- Marie Curie Host Fellowships - Training Site, za 3 študente po eno štipendijo na leto
- Projekt TRACE (FP6-2003-FOOD-2-A); Tracing Food Commodities in Europe
- Projekt IBAAC (An Integrated Biomimetic Approach to Asymmetric Catalysis)
- Projekt COST D2 (New fluoruous media and processes for cleaner and safer chemistry)
- Bilateralni projekt v okviru slovensko - indijskega programa znanstveno tehnološkega sodelovanja 2004 - 2005 z naslovom "QSAR protituberkuloznih spojin: primerjave statističnih modelov in nevronskih mrež"; nosilca: M. Vračko in M. Bagshi
- Bilateralni projekt v okviru slovensko - makedonskega znanstveno - tehnološkega sodelovanja 2004, 2005 in 2006 z naslovom "Študij relacij med kemijsko strukturo in aktivnostjo molekul, ki inhibirajo HIV-1"; nosilca: Ma. Novič in I. Kuzmanovski

included in the OECD document, which has been proposed from JRC. A draft of the document was presented in the OECD meeting held on December 1, 2005 in Paris, France.

At the end let us present our contribution to IBAAC project, namely the chemo-informatics approach toward modeling and optimization of catalysts for stereo specific hydrogenation. We have incorporated into research work of professor Thomas Ward, who has improved stereo specifics of catalysts (ee%) by means of including metal catalyst into the protein environment. Metal catalyst binds through various intermediate parts of molecules (intermediate) on biotin, which has very high affinity to avidin and streptavidin. Our task was to find the position (3D atom coordinates) of each prepared catalyst in the protein binding pocket using "Autodock" software. Because the protein appears as a *doublet of the doublet*, the task was much more demanding. In the future we have the intention, with the help of structural descriptors of the complex metal-ligand-protein of series of catalysts, to optimize the structure of intermediates and also the possible mutations on the protein to improve ee% of chemical reaction.

COLLABORATION WITH THE INDUSTRY

- Lek Pharmaceuticals, d.d., Ljubljana, Slovenia

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:

- Marie Curie Host Fellowships - Training Site, for 3 years, 1 student each yearContract

POMEMBNEJŠI INŠTRUMENTI IN DRUGA OPREMA

- Računalniška učilnica s 30 sedeži in 16 osebnimi računalniki
- DIONEX-DX500 ionski kromatograf z novim avtomatskim vzorčevalnikom
- Project TRACE (FP6-2003-FOOD-2-A) (Tracing Food Commodities in Europe)
- Projekt IBAAC (An Integrated Biomimetic Approach to Asymmetric Catalysis)
- Project COST D29 (New fluoruous media and processes for cleaner and safer chemistry)
- Bilateral project 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: M. Vračko and M. Bagshi
- Bilateral project in the frame of Scientific and technological cooperation between R Slovenia and R Macedonia for the period 2004 - 2006 entitled "Quantitative Structure-Activity Relationship Studies of HIV-1 Inhibitor Molecules"; principal investigators: Ma. Novič and I. Kuzmanovski

IMPORTANT INSTRUMENTS

- Computer supported class-room with 30 seats and 16 PCs
- DIONEX-DX500 ion chromatograph with new autosampler

L04

Laboratorij za analizno kemijo

Analytical Chemistry Laboratory



VODJA / HEAD

Dr. Božidar Ogorevc

RAZISKOVALCI / RESEARCHERS

Dr. Bojan Budič

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Dr. Samo Hočevar

Dr. Miroslav Kovačević

Doc. dr. Milko Novič

Dr. Boštjan Podkrajšek (do / until 30. 6.)

Dr. Janja Turšič

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Marija Slavec

Lea Mauko (od / from november)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Nuša Verbič

Breda Novak

Lidija Živec (polovični del. čas / part time)

Vesna Lenarčič (krajši del. čas / part time)

PODOKTORSKA GOSTJA / POSTDOCTORAL FELLOW

Dr. Emily A. Hutton, Irska / Ireland (do / until 31. 8.)

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

Helena Radič (od / from september)

Suzana Šalinger (od / from september)



PODROČJA DEJAVNOSTI

Področje raziskovalne dejavnosti Laboratorija za analizno kemijo je "analitika in kemijska karakterizacija materialov in procesov" in obsega študij in razvoj sodobnih analiznih metodologij in orodij za analizo (sledov) in določevanje kemijskih vrst 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 L04 zajema tudi pogodbeno delo in

RESEARCH ACTIVITIES

The Analytical Chemistry Laboratory's field of research is analytics and 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, etc. 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 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

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 mnogih anorganskih in organskih ionov ter drugih zvrsti.

Več informacij na naši spletni strani: <http://www.ki.si/slo/Organiziranost/L04/index.html>

BIBLIOGRAFIJA

- 15 izvirnih znanstvenih člankov
- 2 intervjuja
- 1 drugi članek ali sestavek
- 9 objavljenih znanstvenih prispevkov na konferencah
- 32 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 predavanje na tuji univerzi
- 2 končni poročili o rezultatih raziskav
- 8 elaboratov, predštudij, študij

GLAVNI DOSEŽKI V LETU 2005

- V okviru bilateralnega sodelovanja s prof. Glassom iz Velike Britanije in sodelavci iz Politehnikе Nova Gorica smo izvedli študijo, v kateri smo uporabili metodi XANES in EXAFS, da bi pridobili informacijo o molekularni obliki arzena v vzorcih odpadkov iz kalcinacije arzenove rude v neposredni bližini žgalnih peči v Cornwallu in s tem povezano potencialno nevarnost za okolje. Dokazali smo, da je mobilnost arzena veliko večja kot se je doslej domnevalo, saj medatomske razdalje med As-Fe in As-Al ter koordinacijska števila kažejo, da je arzenat v prsti s teh odlagališč prisoten tako v obliki amorfnih ali slabo kristaliziranih železovih hidroksidov (najverjetneje FeAsO_4) kot tudi adsorbiran na aluminijeve okside in/ali hidrokside ter alumosilikate kot je npr. glina.
- Razvili smo teoretični model za izračun maksimalne ekstraktibilnosti kovin iz prsti ali sedimentov za določeno raztopino (ekstraktant), ki je osnovan na predpostavki veljavnosti Langmuirjeve izoterme. Uporabnost

emphasis on development and adaptation of methods and analysis of all kind of samples (environmental, industrial, biological) and determination of practically all elements of the periodic table as well as many inorganic and organic ions.

More information is available at: <http://www.ki.si/Eng/departments/L04/index.html>

BIBLIOGRAPHY

- 15 Original Scientific Articles
- 2 Interviews
- 1 Other Article or Component Part
- 9 Published Scientific Conference Contributions
- 32 Published Scientific Conference Contribution Abstracts
- 1 Invited Lecture at Foreign University
- 2 Final Research Reports
- 8 Treatises, Preliminary Studies, Studies

IMPORTANT ACHIEVEMENTS IN 2005

- In the framework of a bilateral cooperation with Prof. Glass (UK) and in collaboration with Nova Gorica Polytechnic, the x-ray absorption spectroscopic methods XANES and EXAFS were used to retrieve arsenic molecular information in the soil from a calciner's residue dump (Cornwall, UK) to get insight in the normally assumed relative safety of such dump sites. It could be proven that the mobility of arsenic may be much higher than expected based on As-Fe and As-Al distances and coordination numbers which strongly suggest that arsenate in the soil is present in two forms, viz. as amorphous or poorly crystalline hydrous oxides of Fe (most likely FeAsO_4) and adsorbed on aluminium (hydr)oxides or aluminosilicates such as clay.
- A theoretical model was developed for retrieval of the maximal extractability of metals from soil or sediment for a user-defined extractant, based on assumption of a Langmuir isotherm. The applicability of the model was illustrated by determining the chemical availability of seven metals in NIST

predlaganega modela smo eksperimentalno dokazali tako, da smo določili kemijsko razpoložljivost sedmih kovin v standardnem referenčnem materialu NIST 8704 (Buffalo river sediment) za 1 mol l⁻¹ NaOAc (pH 5) kot ekstraktant. V študiji smo tudi pokazali na omejitve modela linearne izoterme, ki so ga uporabljali doslej.

- V okviru bilateralnega projekta smo z našim češkim partnerjem razvili elektrodo iz ogljikove paste, ki je modificirana z bizmutovim prahom (Bi-CPE). Ta elektroda je primerna za določevanje nekaterih težkih kovin v sledovih in je še posebej uporabna takrat, ko je *in situ* priprava tankoslojne bizmutove elektrode neprimerna ali celo nemogoča (npr. okoljske meritve, *in vivo* meritve). Poleg tega je Bi-CPE izredno učinkovita pri določevanju v alkalnih medijih, kjer je *in situ* priprava bizmutovih elektrod manj ugodna.
- V sodelovanju z ameriškim partnerjem smo razvili elektrokemijski mikrosenzor za merjenje pomembne biološke spojine dopamin (živčni prenašalec) ob prisotnosti fizioloških koncentracij askorbata. Pripravljen je na osnovi mikroelektrode iz ogljikovega vlakna, ki je modificirana z ogljikovimi nanocevkami. Ta mikrosenzor je primeren za določevanje nizkih koncentracij dopamina v mikrovolumskih vzorcih in na mikro-lokacijah (npr. za *in vivo* meritve)
- Izvedli smo študijo za pripravo in optimizacijo *ex situ* bizmutove tankoslojne mikroelektrode, primerne za uporabo v elektrokemijski mikroanalizi nekaterih toksičnih kovin (npr. kobalta in niklja). Uvedli smo uporabo bromidnih ionov in optimizirali več parametrov, pomembnih pri elektrolitskem nanašanju bizmutovega sloja na površino ogljikovega vlakna. S tem smo dosegli dolgotrajno mehansko in elektrokemijsko stabilnost take mikroelektrode, kar je pomembno za njeno uporabo npr. pri meritvah težkih kovin v (nizkovolumskih) bioloških tekočinah.

reference material 8704 (Buffalo river sediment) using 1 mol l⁻¹ NaOAc (adjusted to pH 5) as an extractant. The limitations of an earlier used linear isotherm model were demonstrated.

- Within the framework of a bilateral project we prepared, in collaboration with our Czech partner, a carbon paste electrode modified with metallic bismuth powder (Bi-CPE) for measurement of ultratrace heavy metals using electrochemical stripping analysis. Its application is particularly convenient in those environments, where the *in situ* preparation of bismuth film electrode is difficult or even impossible (e.g. environmental monitoring, *in vivo* measurements). Moreover, in contrast to the bismuth film electrode, where the formation of bismuth film at higher pH values appears to be less favourable, we demonstrated that the Bi-CPE even allowed measurements in high alkaline media.
- We have developed an electrochemical microsensor for measurement of a significant biological compound, dopamine (a neurotransmitter), in the presence of physiological concentrations of ascorbate. The proposed microsensor is based on a single carbon fiber microelectrode that is modified with carbon nanotubes. This microsensor holds great promise for measurements of dopamine at low levels in micro-volume samples and at micro-locations, i.e. for *in vivo* measurements.
- We have performed an investigation on the preparation and optimization of an *ex situ* bismuth film microelectrode for use in electrochemical microanalysis of some trace toxic metals (e.g. cobalt and nickel). We have introduced the addition of bromide ions and optimized several parameters important in the electrolytic deposition of the bismuth film onto the surface of a carbon fiber. Based on this work we achieved a long-term mechanical and electrochemical stability of the proposed microelectrode, which is very important in applications such as e.g. the meas-

- Dilema o smrti Velikega Vojvode Mirka Petrovića (1820-1867), člana slavne črnogorske dinastije Njegoš, je bila prisotna vse od njegove smrti do danes. Pri razjasnitvi tega vprašanja smo sodelovali z elementno analizo (z uporabo ICP-AES in ICP-MS) vzorcev las Mirka Petrovića in še nekaterih članov dinastije Njegoš. Rezultati študije so pokazali, da vzrok njegove smrti verjetno ni bila zastrupitev, ampak je nastopila zaradi bolezni (kolera).
- V okviru aplikativnega projekta (z EIMV in TEŠ) smo v sodelovanju s prof. Bernerjem (IEP, Dunaj) zasnovali sistem za vzorčevanje delcev na izvoru (dimnik). Osnova sistema je nizkotlačni kaskadni impaktor, ki ločuje delce glede na njihovo velikost v deset velikostnih razredov (0,015-16,0 μm), in je prilagojen meritvam pod ekstremnimi pogoji (visoke temperature in vlaga ter koncentracija delcev). S tem sistemom smo nato opravili prve meritve emisij trdnih delcev na dimniku TEŠ (blok 4, na višini 50 m, Slika 1). Vzoredno smo izpeljali tudi meritve emisij na dveh izbranih lokacijah, ki sta različno oddaljeni od izvora. Zbranim depozitom delcev smo določili masno porazdelitev in jih kemijsko okarakterizirali (določitev elementov pomembnih kot sledilci).
- The uncertainty about the cause of death of Duke Mirko Petrović (1820-1867), a member of a famous Njegoš Dynasty of Montenegro, existed from his death till now. In order to elucidate whether or not he died of natural causes we performed an elemental analysis study (using ICP-AES and ICP-MS) on samples of his hair, and also on hair samples of some other members of the Njegoš family. The results of this study suggested that he was not poisoned but rather died of a disease (cholera).
- In the frame of an applied research project (with EIMV and TEŠ) we designed, in cooperation with Prof. Berner (IEP, Vienna), a special system for sampling aerosol particles directly at the source of emission. The system is based on a low-pressure cascade impactor, which allows size-segregated sampling of particles in the range 0.015-16.0 μm , and can operate under extreme conditions (high temperature, humidity and particle concentrations). Using such a system we performed measurements of emission of aerosol particles at the stack of TEŠ (Block 4, at the height of 50 m, Figure 1) as well as sampling at two



SLIKA 1:

Specialni sistem za vzorčevanje aerosolskih delcev po velikosti (0,015 – 16 μm) na izvoru emisije. Prve meritve emisije delcev na dimniku Termoelektrarne Šoštanj (blok 4, na višini 50 m) so bile izvedene junija 2005.

FIGURE 1:

A special system for sampling size-segregated aerosol particles (0.015 – 16 μm) directly at the source of emission. In June 2005, we successfully performed preliminary measurements of emission of particles at the stack in Thermopower-plant Šoštanj (Block 4, at the height of 50 m).

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V letu 2005 smo sodelovali z več industrijskimi in drugimi partnerji v okviru pogodb ali naročil za razvoj metod oz. kemijsko analizo različnih vzorcev iz proizvodnje ali okolja, ki zahtevajo posebno znanje in izkušnje ter specialno instrumentacijo. Med najpomembnejše industrijske partnerje tovrstnega sodelovanja v letu 2005 sodijo:

- Salonit Anhovo d.d., Deskle; Lek d.d., Ljubljana; Petrol d.d., Ljubljana; Donit Tesnit d.d., Medvode; Pivovarna Union d.d., Ljubljana; Komplast d.o.o., Ljubljana; Fuchs maziva LSL d.o.o., Krška vas; Melamin d.d., Kočevje; Regeneracija d.o.o., Lesce; Eta d.o.o., Cerklje; Belinka Perkemija d.o.o., Ljubljana; Borosol d.o.o., Medvode; Cimos Titan d.o.o., Kamnik; Sagaris d.o.o., Brežice; TE-TOL, d.o.o., Ljubljana; Unichem d.o.o., Vrhnika; Živalski vrt Ljubljana; Nuklearna elektrarna Krško; Pikas d.o.o., Tolmin; Pivovarna Laško idr.

Sodelovanje z neindustrijskimi partnerji v letu 2005 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 Univerze v Ljubljani; Enota za patologijo prehrane in higieno okolja (NVI, Veterinarska fakulteta Univerze v Ljubljani); Inštitut Jožef Stefan, Ljubljana; Zavod za gradbeništvo Slovenije, Ljubljana; Inštitut za hmeljarstvo in pivovarstvo Slovenije, Žalec; Laboratorij za astrofiziko osnovnih delcev in Laboratorij za raziskave v okolju, Politehnika Nova Gorica; Očesna klinika, Medicinska fakulteta Univerze v Ljubljani; Laboratorij za raziskavo možganov, Inštitut za patološko fiziologijo, Medicinska fakulteta Univerze v Ljubljani idr.

V letu 2005 smo nadaljevali z izvajanjem raziskovalno - aplikativnega projekta z naslovom "Vpliv emisijskih virov na onesnaženje zraka s

different locations, which were at different distances from the source. We further performed mass size distribution and chemical characterization of deposits (determination of elements important as tracers).

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

In 2005 we collaborated with numerous industrial and other partners within the framework of contracts, and also service, to conduct elemental analysis in various samples from industrial processes and the environment, 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 2005 comprises:

- Salonit Anhovo d.d., Deskle, Slovenia; Lek d.d., Ljubljana, Slovenia; Petrol d.d., Ljubljana, Slovenia; Donit Tesnit d.d., Medvode, Slovenia; Pivovarna Union d.d., Ljubljana, Slovenia; Komplast d.o.o., Ljubljana, Slovenia; Fuchs maziva LSL d.o.o., Krška vas, Slovenia; Melamin d.d., Kočevje, Slovenia; Regeneracija d.o.o., Lesce, Slovenia; Eta d.o.o., Cerklje, Slovenia; Belinka Perkemija d.o.o., Ljubljana, Slovenia; Borosol d.o.o., Medvode, Slovenia; Cimos Titan d.o.o., Kamnik, Slovenia; Sagaris d.o.o., Brežice, Slovenia; TE-TOL, d.o.o., Ljubljana, Slovenia; Unichem d.o.o., Vrhnika, Slovenia; ZOO Ljubljana, Slovenia; Nuclear Power Plant Krško, Slovenia; Pikas d.o.o., Tolmin, Slovenia; Pivovarna Laško, Slovenia etc.

Collaboration with non-industrial partners in 2005 represented contract and other development and research work with the following partners:

- Agency of the Republic of Slovenia for the Environment, Ljubljana, Slovenia; Electroinstitute Milan Vidmar, Ljubljana, Slovenia; Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia; Unit for

trdnimi delci" v sodelovanju z Elektroinštitutom Milan Vidmar in Termoelektrarno Šoštanj.

MEDNARODNO SODELOVANJE

V letu 2005 so bili sodelavci Laboratorija za analizno kemijo vključeni v naslednje mednarodne projekte:

- INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change"). Program evropske znanstvene fudacije 2004 - 2008; nacionalna koordinatorica in članica vodstvenega odbora: I. Grgić
- COST Action 633 "Particulate Matter: Properties Related to Health Effects", projekt poteka v okviru Evropske znanstvene fundacije 2002 - 2007; nacionalna koordinatorica ter podpredsednica COST 633: J. Turšič
- Bilateralni projekt "Heterogene reakcije atmosferskih aerosolov pri kontroliranih eksperimentalnih pogojih značilnih za meglico - drugi del" v okviru slovensko - avstrijskega znanstvenega sodelovanja 2004 - 2005; partner: R. Hitzemberger, Inštitut za eksperimentalno fiziko, Univerza na Dunaju, Avstrija; nosilka projekta: I. Grgić
- Bilateralni projekt "Novi materiali za elektrokemijsko detekcijo v stripping analizi" v okviru slovensko - češkega znanstvenega sodelovanja 2004 - 2005; partner: K. Vytras, University of Pardubice, Pardubice, Češka; nosilec projekta: B. Ogorevc
- Bilateralni projekt "Študij sestave, strukture in uporabnosti naravnih zeolitov v sistemih za zaščito okolja" v okviru slovensko - hrvaškega znanstvenega sodelovanja 2003 - 2005; partner: Š. Cerjan-Štefanović, Vseučilišče iz Zagreba, Hrvaška; nosilec projekta: Mi. Novič
- Sodelovanje v bilateralnem projektu z naslovom "Safety assessment and remediation strategies for heavily arsenic-contaminated sites" (PSP-21/2005); partner: H. J. Glass, University of Exeter v Cornwallu, Velika Britanija

Pathology of Animal Nutrition and Environmental Hygiene (NVI, Veterinary Faculty, University of Ljubljana, Slovenia); Jozef Stefan Institute, Ljubljana, Slovenia; Slovenian National Building and Civil Engineering Institute, Ljubljana, Slovenia; Laboratory for Astroparticle Physics and Laboratory for Environmental Research, Nova Gorica Polytechnic, Slovenia; Eye Clinic, Medical School, University of Ljubljana, Slovenia; Laboratory for Brain Research, Institute of Pathophysiology, Medical School, University of Ljubljana, Slovenia, etc.

In 2005 we continued carrying out the applied research project entitled "Influence of emission on ambient air pollution by particulate matter" in collaboration with the Electroinstitute Milan Vidmar, Ljubljana, Slovenia and the Thermopower plant Šoštanj, Slovenia.

INTERNATIONAL COLLABORATION

In 2005 the Analytical Chemistry Laboratory team members were involved in the following international projects:

- European Science Foundation Program INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change") 2004 - 2008; national coordinator and member of the Steering Committee: I. Grgić
- COST Action 633 project "Particulate Matter: Properties Related to Health Effects" in the frame of European Science Foundation 2002 - 2007; national representative and vice-chair of COST 633: J. Turšič
- Bilateral project "Heterogeneous Reactions of Atmospheric Aerosols under Controlled Experimental Conditions Typical for Haze - Part 2" in the framework of S&T cooperation between Slovenia and Austria 2004 - 2005; partner: R. Hitzemberger, Institute for Experimental Physics, University of Vienna; principal investigator: I. Grgić
- Bilateral project "New Materials for Electrochemical Detection in Stripping Analysis" in

POMEMBNI INSTRUMENTI IN OPREMA

- Masni spektrometer z induktivno sklopljeno plazmo (ICP-MS, Agilent Technologies, model 7500 ce 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)
- Atomski emisijski spektrometer z induktivno sklopljeno plazmo (ICP-AES, Thermo Jarrell Ash, Model Atomscan 25) opremljen z ultrazvočnim razpršilcem (Cetac, model U-6000 AT)
- Dva sistema za ionsko kromatografijo (IC) s konduktometrično in spektrofotometrično detekcijo
- Pretočno injekcijski analizator (ASIA Ismatec)
- Več modularnih računalniško vodenih elektrokemijskih sistemov (Autolab, Eco Chemie)
- Invertni optični mikroskop (Eclipse, Nikon)
- Oprema za izdelavo mikroelektrod (aparatus za vlečenje kapilar, stereo leča, aparat za brušenje mikroelektrod, mikromanipulator idr.)
- Reakcijska komora za raziskovanje reaktivnosti aerosolskih delcev pod kontroliranimi pogoji
- Oprema za vzorčevanje aerosolov z Bernerjevimi nizkotlačnimi kaskadnimi impaktorji
- Mikrovalovna peč za razklope (MLS 1200 MEGA, Milestone)

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

V tujino:

- J. T. van Elteren je bil na šest tedenskem delovnem obisku pri dr. Masonu na Utrecht University, Nizozemska
- J. Turšič je bila na dveh eno - tedenskih

the framework of S&T cooperation between Slovenia and the Czech Republic 2004 – 2005; partner: K. Vytras, University of Pardubice, Pardubice, Czech Republic; principal investigator: B. Ogorevc

- Bilateral project "Study of Composition, Structure and Application of Natural Zeolites in Environment Protection Systems" in the framework of S&T cooperation between Slovenia and Croatia 2003 -2004; partner: Š. Cerjan-Štefanović, Faculty of Chemical Engineering and Technology, University of Zagreb, Croatia; principal investigator: Mi. Novič
- Collaboration in a bilateral project "Safety assessment and remediation strategies for heavily arsenic-contaminated sites" (PSP-21/2005); partner: H. J. Glass, University of Exeter in Cornwall, United Kingdom

MAJOR EQUIPMENT

- Inductively coupled plasma mass spectrometer (ICP-MS, Agilent Technologies, Model 7500 ce 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, Model Atomscan 25) equipped with ultrasonic nebulizer (Cetac, Model U-6000 AT)
- Two ion chromatography (IC) systems with conductivity and spectrophotometric detection.
- Flow injection analyzer (ASIA Ismatec)
- Several modular computer assisted electrochemical workstations (Autolab, Eco Chemie).
- Inverted optical microscope (Eclipse, Nikon)
- Microelectrode fabrication tools (capillary puller, stereo zoom, microelectrode beveler, micromanipulator, etc.)

- delovnih obiskih na Inštitutu za eksperimentalno fiziko, Univerza na Dunaju, Avstrija
- S. Hočevar je bil na eno - tedenskem delovnem obisku na Department of Analytical Chemistry, University of Pardubice, Pardubice, Češka
- Iz tujine:
- Dr. Emily A. Hutton (Dublin City University, Irska) je končala enoletno podoktorsko usposabljanje v L04 na področju razvoja elektrokemijskih senzorjev in mikrosenzorjev.
 - Michael Beeston iz University of Exeter, Velika Britanija, je bil na večmesečnem delovnem obisku in je pod vodstvom so-mentorja J. T.
- Reaction chamber for the investigation of aerosol particle reactivity under controlled conditions
 - Equipment for aerosol sampling (low-pressure cascade impactors of Berner type)
 - Microwave oven for sample digestion (MLS 1200 MEGA, Milestone)

EDUCATION AND IMPORTANT VISITS

Visits abroad:

- J. T. van Elteren: six - weeks work visit to Dr. Mason, Utrecht University, The Netherlands
- J. Turšič: two one - week work visits to the



SLIKA 2:

Nova velika pridobitev Laboratorija za analizno kemijo: Elementni masni spektrometer z lasersko ablacijo (LA-ICP-MS) je sestavljen iz enote za lasersko ablacijo (levo) in masnega spektrometra z induktivno sklopljeno plazmo (desno). Ta sistem omogoča mikrosondiranje površin trdnih vzorcev z ločljivostjo od 5 do 300 nm ter izdelavo globinskih profilov. Možna je detekcija sledov (do ng/g) večine elementov periodnega sistema.

FIGURE 2:

New important research instrumentation in the Analytical Chemistry Laboratory: An elemental mass spectrometer with laser ablation (LA-ICP-MS), comprising a laser ablation unit (LA, left) and an inductively coupled plasma mass spectrometer (ICP-MS, right). It allows microprobing of surfaces of solid samples with a spatial resolution of 5 to 300 nm and recording of depth profiles. It has the capability to detect traces (down to ng/g) of most of the elements in the periodic table.

van Elterena opravljal raziskovalno delo za doktorsko disertacijo

- Doc. dr. Ivan Švancara iz Univerze v Pardubicah, Češka, je bil v L04 na eno - tedenskem delovnem obisku v okviru bilateralnega projekta
- Prof. Axel Berner iz Inštituta za eksperimentalno fiziko, Univerza na Dunaju, Avstrija, je bil na več krajših delovnih obiskih v zvezi z razvojem posebnega sistema za vzorčevanje zračnih delcev na izvoru

POMEMBNA NABAVA VELIKE RAZISKOVALNE OPREME

V Laboratoriju za analizo kemijo smo v letu 2005 nabavili moderno raziskovalno opremo namenjeno kemijski karakterizaciji trdnih materialov "Elementni masni spektrometer z lasersko ablacijo" (LA-ICP-MS, Slika 2), ki je prvi tovrstni sklopljeni analizni sistem v Sloveniji. Nakup opreme v vrednosti 61 mio SIT so podprli strukturni skladi EU in slovenski partnerji: Ministrstvo za visoko šolstvo, znanost in tehnologijo, Univerza v Ljubljani ter Institut Jožef Stefan.

LA-ICP-MS predstavlja najsodobnejšo raziskovalno tehniko za direktno kemijsko (elementno) karakterizacijo trdnih materialov, ki nudi

Institute for Experimental Physics, University of Vienna, Austria

- S. Hočvar: one - week work visit to the Department of Analytical Chemistry, University of Pardubice, Pardubice, Czech Republic

Visits from abroad:

- Dr. Emily A. Hutton, Dublin City University, Ireland has accomplished a one - year postdoctoral research visit to our Laboratory, working in the area of electrochemical sensors and microsensors
- Mr. Michael Beeston from the University of Exeter, United Kingdom has been on a several months work visit under the supervision of his co-mentor J. T. van Elteren from our Laboratory, to perform a part of his PhD research program
- Asst. Prof. Ivan Švancara from the University of Pardubice, Czech Republic has been on a one - week work visit in the framework of a bilateral project
- Prof. Axel Berner from the Institute of Experimental Physics, University of Vienna, Austria has been on several short - term working visits in connection with the development of a special system for the size-segregated sampling of aerosols at the source of emission



SLIKA 3

Povečana fotografija človeškega lasu po analizi (mikrosondaži) z lasersko ablacijo z vidnimi kraterji, ki jih je izdolbel laserski žarek, čemur je sledila določitev elementov z ICP-MS. Primer za idealno uporabo LA-ICP-MS, ko je na voljo le izredno majhna količina materiala.

FIGURE 3

Optical microscope photograph of a human hair after LA-ICP-MS analysis (microprobing), displaying craters left behind by drilling with the laser beam. This example illustrates that LA-ICP-MS is an ideal technique for elemental microanalysis of very small samples.

raznovrstne in zelo aktualne možnosti uporabe na različnih področjih, kot so npr. geologija, metalurgija, pedologija, razvoj novih materialov, farmacija, forenzika, arheologija, konservatorstvo in restavracijsko, botanika itd. Idealna je v tistih primerih, ko so potrebne meritve sledov elementov (< 0.1%) na površini in v materialu, ko je na voljo le majhna količina materiala (Slika 3), ali pa so vzorci dragoceni, saj se z laserskim žarkom obseva razmeroma majhen del površine vzorca (premer 4 - 300 mm), ki zato ostane praktično nepoškodovan.

IMPORTANT PURCHASE OF MAJOR RESEARCH EQUIPMENT

In 2005 the Analytical Chemistry Laboratory obtained state-of-the-art research equipment that can be used for chemical characterization of solid materials, namely an elemental mass spectrometer with laser ablation unit (LA-ICP-MS, Figure 2), which is the first hyphenated analytical system of its kind in Slovenia. The purchase of this system, with a value of ca. 260,000 Euro, was supported by the EU Structural Funds and by several partners in Slovenia: The Ministry of Higher Education, Science and Technology, the Jožef Stefan Institute and the Faculty of Chemistry and Chemical Technology (UL).

LA-ICP-MS is a frontier research technique for direct chemical (elemental) characterization of solid materials that offers versatile and topical measurement options in different fields such as geology, metallurgy, pedology, material science, pharmaceutical development, forensics, archeology, conservation and restoration, botanics, etc. It is ideal for measurements of trace elements (< 0.1%) at the surface and in the bulk of a solid material, and when only a small amount of a sample is available (Figure 3) or in situations when precious samples have to be analysed, as the irradiation with the laser beam affects only a very small part (diameter of 4 - 300 mm) of the surface of a valuable object, which is therefore left practically undamaged.

L05

Laboratorij za kemijo,
biologijo in tehnologijo vod

Laboratory for Chemistry,
Biology and Technology of Water



VODJA / HEAD
Prof. dr. Milenko Roš

RAZISKOVALCI / RESEARCHERS

Dr. Magda Cotman
Dr. Andreja Drolc
Dr. Tatjana Tišler
Dr. Janez Vrtovšek
Prof. dr. Jana Zagorc Končan
Dr. Gregor D. Zupančič

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Anita Jemec
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Emil Meden
Matjaž Omerzel

PRIPRAVNIKI / TRAINEES

Melissa Maria Lavdas, Švica / Switzerland
(IAESTE)
Tanja Urh (3 mesečna visokošolska praksa / 3
months)
Melita Rupnik (3 mesečna visokošolska praksa /
3 months)



PODROČJA DEJAVNOSTI

a) Raziskovalni program:

- Integralni pristop k preprečevanju onesnaževanja voda - (MVŠZ)

b) Raziskovalni projekti:

- Meroslovna sledljivost v kemiji - vloga referenčnih materialov in referenčnih merjenj (MVŠZT) - nosilka: A. Drolc
- Razvoj postopka za stabilizacijo, mineralizacijo in higienizacijo blata iz malih čistilnih naprav - nosilec: G. D. Zupančič
- Kemijsko in biološko sledenje neonukleotidov in njihovega vpliva v okolju; nosilka; P. Trebše, Politehnika Nova Gorica
- Biološki testi za ugotavljanje toksičnosti in genotoksičnosti vode, zemlje in hrane; nosilka; R. Marinšek Logar, Biotehniška fakulteta
- Razvoj celovitega sistema za ugotavljanje toksičnosti in genotoksičnosti v zemlji, vodi in hrani v soglasju s smernicami EU; nosilka; R. Marinšek Logar, Biotehniška fakulteta

c) Slovenski ekološki grozd

RESEARCH ACTIVITIES

a) Research Programme:

- Integrated approach to water pollution prevention

b) Research Projects:

- Metrological traceability in chemistry - role of reference materials and reference measurements - principal researcher: A. Drolc,
- Procedure development for stabilization, mineralization and hygienization of sludge from small biological wastewater treatment plants - principal researcher: G. D. Zupančič
- Chemical and biological monitoring of neonicotinoids and their impact assessment in the environment (principal researcher; P. Trebše, Nova Gorica Politehnic, Slovenia)
- Biological tests for toxicity and genotoxicity determination in water, soil, and food (principal researcher; R. Marinšek Logar, Biotechnical faculty, University of Ljubljana, Slovenia)
- Development of an integrated system for assessment of toxicity and genotoxicity in soil, water and food in concordance with

Sodelovanje na projektih:

- Razvoj in avtomatizacija SBR
- Raziskave mineralizacije blata iz bioloških čistilnih naprav na pilotni napravi

d) Center odličnosti - okoljske tehnologije

Sodelovanje na pripravi projektov:

- Razvoj novih metod za čiščenje odpadnih vod v SBR in
- Biološka stabilizacija blata

BIBLIOGRAFIJA

- 4 izvorni znanstveni članki
- 2 strokovna članka
- 1 intervju
- 2 druga članka ali sestavka
- 1 univerzitetni ali visokošolski učbenik z recenzijo
- 2 drugi učni gradivi
- 1 priročnik, slovar leksikon, atlas, zemljevid
- 5 objavljenih strokovnih prispevkov na konferencah (vabljeni predavanja)
- 13 objavljenih znanstvenih prispevkov na konferencah
- 15 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 predavanje na tuji univerzi
- 1 prispevek na konferenci brez natisa
- 3 vabljeni predavanja na konferenci brez natisa
- 8 končnih poročil o rezultatih raziskav
- 2 elaborata, predštudiji, študiji
- 3 izvedenska mnenja, arbitražne odločbe
- 2 diplomi
- 2 magisterija

GLAVNI DOSEŽKI V LETU 2005

- Postavitev pilotne naprave za obdelavo blata na Čistilni napravi v Velenju skupaj s firmo Esotech d.d., Velenje in Komunalnim podjetjem iz Velenja; s pomočjo tehnologije razvite na Kemijskem Inštitutu in patentirane (Postopek in naprava za stabilizacijo in mineralizacijo blata iz naprav za čiščenje odpadne vode v termofilnem temperaturnem območju : patent št. 21318), bomo testirali

the EU directives (principal researcher; R. Marinšek Logar, Biotechnical faculty, University of Ljubljana, Slovenia)

c) Slovenian Ecological Cluster

Co - operation on the following sub - projects:

- Development and automation of SBR
- Research on mineralization of sludge from biological wastewater treatment plants

d) Centre of Excellence

Co - operation on the following sub - projects:

- Development of new methods on wastewater treatment in the SBR
- Biological stabilization of sludge

BIBLIOGRAPHY

- 4 Original Scientific Articles
- 2 Professional Articles
- 1 Interview
- 2 Other Articles or Component Parts
- 1 Reviewed University and Academic Textbook
- 2 Other Educational Material
- 1 Manual, Dictionary, Lexicon, Atlas, Map
- 5 Published Professional Conference Contributions (Invited Lecture)
- 13 Published Scientific Conference Contributions
- 15 Published Scientific Conference Contribution Abstracts
- 1 Invited Lecture at a Foreign University
- 1 Unpublished Conference Contribution
- 3 Unpublished Invited Lectures at a Conference
- 8 Final Research Reports
- 2 Treatises, Preliminary Studies, Studies
- 3 Expertises, Arbitration Decisions
- 2 Undergraduate Theses
- 2 Master's Theses

IMPORTANT ACHIEVEMENTS IN 2005

- Construction of pilot plant for two stage sludge digestion in wastewater treatment plant in Velenje, Slovenia; with use of pat-

pogoje obratovanja in s pomočjo podatkov bodo v Velenju na čistilni napravi postavili obdelavo blata po naši tehnologiji

- Rešitev problematike odpadnih voda in gošč Pivovarne Union, Ljubljana z našo tehnologijo
- Razvoj postopka za odstranitev sekundarnega amonija na bioloških čistilnih napravah s pomočjo prirejene aerobne stabilizacije blata
- Na osnovi preizkusov v pilotnem SBR je bila izbrana tehnologija čiščenja in pridobljeni podatki za dimenzioniranje industrijske čistilne naprave za obdelavo odpadne vode lesne industrije; s pilotnimi preizkusi smo potrdili tudi učinkovitost delovanja SBR v primeru, če odpadne vode vsebujejo specifične organske snovi, ki v vodnem ekosistemu delujejo kot motilci endokrinega sistema
- V pilotnem SBR smo opravili osnovne preizkuse z visoko koncentracijo biomase (>10 gSS/l), ki hkrati ohrani odlične lastnosti usedanja in učinkovitega prezračevanja
- Vzdrževanje sistema kakovosti (akreditacija) po standardu SIST EN ISO/IEC 17025
- Izvedba dveh medlaboratorijskih preskušanj
- Vključitev v bazo EPTIS (BAM Nemčija)
- Izvedba mednarodne delavnice TrainMiC, skupaj z JRC-IRMM Belgija
- Razvoj postopkov za določanje subletalnih vplivov strupenih snovi na aktivnosti biokemijskih biomarkerjev v rakah vodne bolhe (*Daphnia magna*) po kratkotrajni izpostavljenosti
- Uvajanje biološkega preskusa za določanje prisotnosti hormonskih motilcev v vodi s kvasovko *Sacharomyces cerevisiae*
- Optimizacija ATP metode za določanje strupenosti dotokov na biološke čistilne naprave

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Ministrstvo za okolje in prostor - Agencija RS za okolje
- Nuklearna elektrarna Krško, Krško

ented technology (*Procedure and device for thermophilic temperature range sludge stabilization and mineralization: patent No. 21318*) developed at the National institute of Chemistry, the operational conditions will be tested and used for full scale digester construction

- Developing wastewater and slurry treatment technology for Union Brewery, Ljubljana, Slovenia
- Development of procedure of secondary ammonia removal in wastewater treatment plants utilizing modified aerobic digestion
- Design parameters for the industrial wastewater (wood technology) treatment plant were obtained with the experiments in the pilot sequencing batch reactor (SBR) system; pilot experiments also showed, that the SBR is one of the established technologies which could provide optimal conditions for the treatment of wastewater with endocrine disrupting chemical (nonylphenol) due to its flexible operation and efficient selection of desired microbial population
- Basic pilot experiments were performed in the SBR with high biomass concentration (> 10 gSS/L)
- Support to quality system (accreditation) according to requirements of standard ISO/IEC 17025
- Providing two distributions of ILC
- Register our ILC Scheme on EPTIS database
- Realization of international workshop TrainMiC together with JRC-IRMM, Geel, Belgium
- Introduction of new methods for determination of sublethal effects of pollutants on biochemical biomarkers in water flea *Daphnia magna* after acute exposure
- Development of protocols for measuring endocrine disruptors in waters with *Sacharomyces cerevisiae*
- Optimization of method with adenosine tri-

- Zavod za gradbeništvo Slovenije (ZAG), Ljubljana
- Komunalna Energetika Ljubljana (KEL), Ljubljana
- Urad za meroslovje Republike Slovenije, Ljubljana
- Komunalno Podjetje Velenje, Velenje
- Pivovarna Union, Ljubljana
- Esotech d.d., Velenje
- Dr. Duhovnik d.o.o., Seničica
- Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani
- Biotehniška fakulteta: Oddelek za biologijo in Oddelek za zootehniko, Univerza v Ljubljani
- Veterinarska fakulteta, Univerza v Ljubljani
- Inštitut za fizikalno biologijo, Grosuplje
- Politehnika, Nova Gorica

MEDNARODNO SODELOVANJE

- 5. okvirni program (OP): CoEPT-Comparability of the Operating and Evaluation Protocols

phosphate (ATP) for toxicity evaluation of influents to wastewater treatment plants

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Ministry of Environment and Spatial planning
 - Agency for the Environment, Slovenia
- Nuclear Power Plant, Krško, Slovenia
- Slovenian Building and Civil Engineering Institute, Ljubljana, Slovenia
- Public Utility Energetics, Ljubljana, Slovenia
- Metrological institute of Republic of Slovenia, Ljubljana, Slovenia
- Municipality of Velenje, Slovenia
- Brewery Union, Ljubljana, Slovenia
- Esotech d.d., Velenje, Slovenia
- Dr. Duhovnik d.o.o., Seničica, Slovenia
- Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia
- Biotechnical Faculty: Department of Biology and Zootechnical Department, University of Ljubljana, Slovenia



SLIKA 1:
Pilotna naprava za obdelavo blata

FIGURE 1:
Pilot plant for sludge treatment

- of European Proficiency Testing Schemes in the Chemistry Sector
- Projekt 6. OP: European Analytical Quality Control in Support of Water Information System for Europe (EAQC-WISE); Kemijski inštitut je član ožjega vodstva projekta (Scientific council) in vodja delovnega področja
- Projekt EUROMET Support Programme for Metrology in Chemistry in EU Candidate Countries (TrainMiC – Training in Metrology in Chemistry)

POMEMBNI INŠTRUMENTI IN OPREMA

- Štirje kombinirani anaerobno-anoksično-aerobni reaktorji (KI)

- Veterinary Faculty, University of Ljubljana, Slovenia
- Institute of Physical Biology, Grosuplje, Slovenia
- Nova Gorica Polytechnic, Nova Gorica, Slovenia

INTERNATIONAL COLLABORATION

- CoEPT-Comparability of the Operating and Evaluation Protocols of European Proficiency Testing Schemes in the Chemistry Sector
- Project 6. FP (Contract No. 022603) European Analytical Quality Control in Support of Water Information System for Europe (EAQC-WISE); National Institute of Chemis-



SLIKA 2:
Anaerobni reaktor za obdelavo blata

FIGURE 2:
Anaerobic reactor for sludge treatment

- Avtomatizirani šaržni biološki reaktor (ŠBR)
- LUMIS-TOX aparatura (dr. Lange)
- Avtomatizirani respirometer (MICRO-Oxymax 6.0, Columbus Instruments)
- Ionski kromatograf (DIONEX 120) s samodejnim vzorčevalnikom (DIONEX AS 3500)
- Kjeltec sistem 2300 Autosystem II (FOSS Tecator) za razklop in določanje Kjeldahlovega dušika
- TOC analizator TOC-5000A (SHIMADZU)
- Laboratorijski modeli rek
- Spektrofotometer Lambda 20 (Perkin-Elmer)
- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector
- Štirje laboratorijski modeli bioloških čistilnih naprav
- Anaerobni reaktor z opremo
- Čitalec mikrotiterskih plošč (Bio-tek, MicroWave XS)

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- M. Roš: priprava modula "Sampling" v okviru TrainMiC (Training of Measurements in Chemistry) projekta, na Inštitutu za Referenčne Materiale in Meroslovje, Geel, Belgija (JRC-IRMM) - 3 mesece
- T. Tišler: delovni obisk na Institute of Physical Chemistry, Faculty of Physics and Chemistry, University of Tartu, Tartu, Estonia
- A. Jemec: udeležba delavnice Second Workshop on Comparative Aspects of Oxidative Stress in Biological Systems, La Paz, Baja California Sur, Mexico
- Izvajanje magistrskih in diplomskih del, ki jih vodita M. Roš in J. Zagorc-Končan
- Izvajanje vaj za Politehniko Nova Gorica, ki jih vodi M. Roš v sodelovanju z A. Drolc
- Sodelovanje pri vajah na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani (A. Drolc, M. Cotman)
- Sodelovanje pri izvedbi diplomskih in doktorskih del z Biotehniško fakulteto

try is member of scientific council of the project and Work Package leader

- Project EUROMET (No. 693) Support Programme for Metrology in Chemistry in EU Candidate Countries (TrainMiC – Training in Metrology in Chemistry)

MAJOR EQUIPMENT

- Four combined anaerobic-anoxic-aerobic laboratory pilot plant reactors (NIC)
- Automated sequencing batch reactor (SBR)
- LUMIS-TOX apparatus (dr. Lange)
- Automated respirometer (MICRO-Oxymax 6.0, Columbus Instruments)
- Ion chromatograph (DIONEX 120) with automatic sampler (DIONEX AS 3500)
- Kjeltec system 2300 Autosystem II (FOSS Tecator) for Kjeldahl N determination
- TOC-5000A, SHIMADZU for determination of Total Organic Carbon (TOC)
- Laboratory river models
- Spectrophotometer Lambda 20 (Perkin-Elmer)
- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector
- Four laboratory pilot plant wastewater treatment plants
- Anaerobic reactor with equipment
- Micro-plate reader (Bio-tek, MicroWave XS)

EDUCATION AND IMPORTANT VISITS

- M. Roš: composition of the module "Sampling in the frame of TrainMiC (Training of Measurements in Chemistry) project at the Institute for Reference Materials and Measurements (JRC-IRMM), Geel, Belgium - 3 months
- T. Tišler: visit to Institute of Physical Chemistry, Faculty of Physics and Chemistry, University of Tartu, Tartu, Estonia
- A. Jemec: participation in Second Workshop on Comparative Aspects of Oxidative Stress

- Univerze v Ljubljani, Oddelek za zootehniko in Oddelek za biologijo
- Soorganizacija delavnice TraiMic, skupaj z JRC-IRMM, Geel, Belgija
 - Soorganizacija konference z mednarodno udeležbo, VODNI DNEVI 2005, kjer so sodelavci laboratorija sodelovali kot predavatelji
- Iz tujine:
- Prof. dr. Kees van Gestel, Institute of Ecological Science, Vrije Universiteit, Amsterdam, The Netherlands
 - Prof. dr. Peter Wilderer, Institute for Water and Waste Management, TU Muenchen, Garching, Germany
 - Strokovna praksa v organizaciji IAESTE Ljubljana, praktikantka Melissa Maria Lavdas in Biological Systems, La Paz, Baja California Sur, Mexico
 - Carrying out of diploma works, master's works and doctoral thesis conducted by J. Zagorc Končan and M. Roš in co-operation with A. Drolc and M. Cotman
 - Practice performing for the Nova Gorica Polytechnic, Slovenia, conducted by M. Roš, assistant for practice is A. Drolc
 - Cooperation with Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia
 - Train MiC workshop organization in collaboration with JRC-IRMM, Geel, Belgium
 - Co - organization of the Conference with international participation, WATER DAYS 2005, Portorož, Slovenia



SLIKA 3:
KI Nosilec referenčnega etalona

FIGURE 3:
NIC Holder of the reference standard

(Swiss Federal Institute of Technology, Zurich, Švica)

POSEBNI DOSEŽEK

Imenovanje Kemijskega inštituta za nosilca referenčnega etalona za enoto mol, področje varovanje okolja, vrsta vzorca odpadne vode.

- Cooperation with Biotechnical faculty: Zootechnical Department and Department of Biology, University of Ljubljana, Slovenia in undergraduate and postgraduate theses

Visit from abroad:

- Prof. Dr. Kees van Gestel, Institute of Ecological Science, Vrije Universiteit, Amsterdam, The Netherlands
- Prof. Dr. Peter Wilderer, Institute for water and waste management, TU Muenchen, Garching, Germany
- Student training: Melissa Maria Lavdas, Swiss Federal Institute of Technology, Zurich, Switzerland, organized by the IAESTE Ljubljana, Slovenia

SPECIAL ACHIEVEMENT

Authorization of the National Institute of Chemistry as holder of reference standard for the unit mol, area of environmental protection, type of sample wastewater.

L06

Laboratorij za prehrambeno kemijo

Laboratory for Food Chemistry



VODJA / HEAD
Dr. Mirko Prošek

RAZISKOVALCI / RESEARCHERS

Dr. Alenka Golc-Wondra
Dr. Breda Simonovska
Dr. Andrej Šmidovnik
Dr. Irena Vovk

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Maja Fir
Mitja Križman
Brigita Lapornik
Mitja Martelanc
Kajetan Trošt

TEHNIČNO OSEBJE / TECHNICAL STAFF

Mateja Puklavec

PRIPRAVNIKI / TRAINEES

Tina Celestina
Barbara Kapun



PODROČJA DEJAVNOSTI

Raziskovalno delo Laboratorija za prehrabeno kemijo (L06) je usmerjeno na področje znanstvenega načrtovanja izdelkov in prehranskih dodatkov, aditivov za zdravo prehrano. Delo poteka v petih podskupinah in sicer na:

- razvoju novih prehrabnih izdelkov in prehranskih dodatkov s funkcionalnimi lastnostmi
- priprava in vrednotenje specialne prehrane in prehrabni inženiring
- določanju spojin naravnega izvora s sodobnimi kromatografskimi in spektroskopskimi tehnikami
- razvoju in validaciji novih analiznih metod in analiznih tehnik
- preprečevanju kemijskih tveganj z upoštevanjem dobrih praks (GLP in GMP) pri razvoju in validaciji analiznih metod, tehnoloških validacijah, validacijah čiščenja in HCCAPa.

BIBLIOGRAFIJA

- 8 izvirmih znanstvenih člankov

RESEARCH ACTIVITIES

Research activities are oriented into the scientifically designed food for healthy nutrition. They are divided in 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 hazard in food production according to GLP, GMP and HCCAP

BIBLIOGRAPHY

- 8 Original Scientific Articles
2 Other Articles or Component Parts
1 Manual, Dictionary, Lexicon, Atlas, Map
7 Published Scientific Conference Contributions
11 Published Scientific Conference Contribution Abstracts

- | | | | |
|----|---|---|---|
| 2 | druga članka ali sestavka | 1 | Published Professional Conference Contribution Abstract |
| 1 | priročnik, slovar leksikon, atlas, zemljevid | 2 | Patent Applications |
| 7 | objavljenih znanstvenih prispevkov na konferencah | 1 | Patent |
| 11 | objavljenih povzetkov znanstvenih prispevkov na konferencah | 1 | Final Research Report |
| 1 | objavljeni povzetek strokovnega prispevka na konferenci | 1 | Treatise, Preliminary Study, Study |
| 2 | patentni prijavi | 7 | Undergraduate Theses |
| 1 | patent | 2 | Doctoral Dissertations |
| 1 | končno poročilo o rezultatih raziskav | | |
| 1 | elaborat, predštudija, študija | | |
| 7 | diplom | | |
| 2 | doktorata | | |

GLAVNI DOSEŽKI V LETU 2005

- Raziskave so potekale na področju prehrane in analize kemije in v sodelovanju z zunanjimi partnerji pri razvoju novih farmacevtskih izdelkov in učinkovin. Razvojno raziskovalne naloge so bile vezane na razvoj, optimizacijo, validacijo in uporabo novih 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. Tako smo razvili in validirali analize metode za kvantitativno vrednotenje holesterola, raznih antioksidantov, vitaminov, provitaminov itd. Na zahtevo inšpekcijskih služb smo določevali vsebnost THC v industrijski konoplji pridelani v Sloveniji. Skupaj z Veterinarsko fakulteto Univerze v Ljubljani smo razvili metodo za kvantitativno vrednotenje slakorjev v plazmi in s to metodo pri psih ugotavljali poškodovanost črevesne sluznice po zaužitju nekaterih zdravil. Razvili smo analizo metodo za določevanje vsebnosti aminokislin v gojiščih, pripravljenih za umetno oplo-

IMPORTANT ACHIEVEMENTS IN 2005

- Activities in L06 were directed to research in food and analytical chemistry and together with partners from industry on evaluation of new pharmaceutical products and active substances. Our research projects were oriented into 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 quantitative determination of cholesterol, antioxidants, vitamins and provitamins.
- Together with Veterinary clinic, Ljubljana, Slovenia, we developed a new analytical method for quantitative evaluation of sugars in blood. Method was successfully used for evaluation of damages produced by some pharmaceutical products on dogs intestines.
- As a part of Food engineering project a new analytical method for quantitative evaluation of amino acids in a nutrient drop prepared for artificial insemination was developed.
- Studies of vegetable oils were focused on preparation and chemical characterisation of new food additives with antioxidant activities. Our additives control the oxidation of oils and products with certain amount of fat (mayonnaises, cream, milk etc.) at higher temperatures and during storage time.

- jevanje. Metoda služi vrednotenju parametrov, ki vplivajo na uspešnost ali neuspešnost oploditve.
- Pripravili in ovrednotili smo prehranske dodatke z antioksidacijskimi lastnostmi, ki pri termični obdelavi in skladiščenju preprečujejo oksidacijski razpad jedilnih olj. Pričakujemo, da bodo te učinkovine zagotavljale kontrolirano stabilnost olj in drugih izdelkov na bazi maščob (majoneza, smetana, mleko, itd).
 - Dokončali smo projekt »Sušilnik za programirano sušenje TLC plošč«. Izbrali smo ustreznega proizvajalca, to je podjetje Iskra PIO d.o.o. iz Šentjerneja in skupaj z njim smo pričeli tržiti izdelek. Sušilnik je pri uporabnikih dobil zelo pohvalne ocene, ker omogoča sušenje v zaprtih in kontroliranih pogojih in s tem istočasno izboljša ponovljivost analiznih meritev in poveča požarno varnost. Izdelek ima slovenski patent in je v fazi patentiranja v nekaterih evropskih državah.
 - Za vodotopno obliko koencima Q10 (CoQ10) smo v letu 2005 vložili mednarodno patentno prijavo PCT/SI2005/000013 in zanjo v Sloveniji že prejeli patent št. SI 21807. Za proizvodnjo in trženje tega izdelka smo sklenili pogodbo s podjetjem Valens Int. d.o.o., Ljubljana, ki je pričel s trženjem vodotopnega CoQ10 pod zaščitno znamko Q10Vital. Sodelovali smo pri pripravi mednarodnega simpozija »Dan koencima Q10«, ki je potekal 10. novembra 2005 v Ljubljani. Simpozija se je udeležilo približno 100 domačih in tujih udeležencev. Na simpoziju smo predstavili vlogo koencima Q10 v človeškem organizmu in prednost našega izdelka v primerjavi z nevodotopnimi in vodotopnimi oblikami tujih proizvajalcev.
 - Pripravili smo pilotno proizvodnjo vodotopnega Q10. Ob tem, da so na trgu že prvi proizvodi narejeni po naši licenci, smo nadaljevali z razvojem in testiranjem novih prehrabnih izdelkov. Pripravili smo mleko, jogurt, kefir, čokoladne izdelke, sadne sokove in celo mineralno vodo obogateno s CoQ10.
- The project »Programmable TLC dryer« was completed and the firm PIO d.o.o., Šentjernej, Slovenia was selected as a producer of commercially available instrument.
 - The international patent application No. PCT/SI2005/000013 was submitted for our water soluble form of Coenzyme Q10 and the Slovenian patent No. SI 21807 was granted for the same. Together with our partner Valens Int. d.o.o., Ljubljana, Slovenia, we started to sell our product under the name Q10Vital. We co-organised the International symposium on Q10, which took place in Ljubljana on 10th November 2005. Nearly 100 participants attended this symposium. Our group presented the role of Q10 in human body and advantages of our water soluble form in comparison to other products on the market.
 - We succeeded in preparing a pilot production of water-soluble Q10. While products made using our licence are already on the market, we have continued with the development and testing of new food items. Milk, yogurt, kefir, chocolate products, fruit juices and even mineral water were enriched with coenzyme Q10. All products were then characterized for their chemical and organoleptic properties, as well as stability. In addition, we developed a synthesis for cyclodextrin complexes with new substances and continued the search for acceptable carriers for the water-soluble CoQ10 preparation.
 - The stability of polyphenols in juices made from blackcurrant using different maceration methods was evaluated. Concentrates from blackcurrant were also added to strawberry juices in order to enrich their colour and antioxidant activity, especially during storage at room temperature. After processing and during the storage, these new products were tested. The content of total polyphenols, anthocyanins, antioxidant activity, vitamin C and individual anthocyanins, flavonols and phenolic acids were measured. Strawberry

Izdelke smo kemijsko in organoleptično ovrednotili in jim določili stabilnost. Istočasno smo pripravljali sintezo ciklodekstrinskih kompleksov z novimi substancami in iskali primerne nosilce za pripravo vodotopnih oblik CoQ10.

- Spremljali smo stabilnost polifenolov v določenih časovnih obdobjih v sokovih iz plodov črnega ribeza, pripravljenih z različnimi načini predelave. V sokovih in koncentratih smo spremljali vsebnost skupnih polifenolov, skupnih antocianov, antioksidativno učinkovitost, vsebnost vitamina C, identificirali in določili vsebnost posameznih antocianinov, flavonolov in fenolnih kislin. Koncentrate smo dodajali v jagodni nektar v izbrani koncentraciji z namenom izboljšati barvo, antioksidativno učinkovitost, predvsem pa stabilnost barve jagodnega nektarja med staranjem na sobni temperaturi. Nektarji z dodatki so imeli večjo antioksidativno učinkovitost, spremenjeno

juices with added concentrates had higher antioxidant activity, higher colour intensity, a red coloured hue, and more vitamin C. All juices with added supplements were scored better than juices without addition, at the beginning and after storage. Now we are looking for the agreement with food manufacturers for application of our additives.

- Our activities within the European project TOM were focused on the isolation of biologically active compounds from the solid residue of the tomato processing industry. In different CO₂ extracts of tomato waste material we found an appreciable content of triterpenoids, from which we succeeded to identify and approximately quantify amyirin. We developed new extraction, fractionation and purification procedure for the isolation of the enzymes pectin methylesterase (PME) and polygalacturonase (PG) from fresh tomato fruit. One of the main forms of tomato PME that is applicable to the food industry



SLIKA 1

Obisk prof. G. P. Littaruja in dr. Jose L. Quilesa na Kemijskem inštitutu

FIGURE 1

Visit of Prof. G. P. Littaru and Dr. Jose L. Quiles at the National Institute of Chemistry

intenziteto in ton barve, več vitamina C, poleg antocianinov, značilnih za jagodni nektar, so vsebovali še antocianine črnega ribeza. Med staranjem so se vsebnosti merjenih parametrov v nektarjih z dodatki koncentratov bolje ohranile, predvsem Pg3G, značilen za barvo jagode. Senzorično so bili takoj in po staranju bolje ocenjeni nektarji z dodanimi koncentratami. Sedaj se dogovarjamo še za industrijsko uporabo pripravljenih koncentratov.

- V okviru EU projekta TOM so bile naše raziskave usmerjene v izolacijo biološko aktivnih spojin prisotnih v odpadkih iz proizvodnje izdelkov iz paradižnika. Ugotovili smo, da vzorci vsebujejo precej triterpenoidov, od katerih smo uspeli identificirati in približno ovrednotiti amirin v CO₂ ekstraktih ostankov po predelavi paradižnika. Razvili smo nov postopek ekstrakcije in izolacije dveh encimov pektin metilesteraze (PME) in poligalakturonaze (PG) iz paradižnika. Izolirali smo eno od oblik PG in eno od oblik PME, ki za svoje delovanje ne potrebuje natrijevega klorida in bi jo lahko uporabili v prehrabeni industriji. Za izolacijo so bile ključnega pomena kratke monolitne kolone (CIM® diski) podjetja BIA Separations d.o.o., Ljubljana. Oba encima (PG in PME), ki smo ju uspeli izolirati čista in z ohranjeno aktivnostjo, je nizozemsko podjetje Catchmabs uporabilo za generiranje monoklonskih protiteles iMab in nato za razvoj metode za direktno izolacijo teh encimov iz ekstrakta paradižnika z afinitetno kromatografijo.
- Raziskovali smo tudi, kakšen vir karotenoida likopena (rdečega barvila zrelega paradižnika) so različni komercialni izdelki na slovenskem tržišču (pasirani paradižnik, kečapi, dvojni koncentrat, prehranski dodatek likopena v obliki tablet, itd). Ekstrakcija likopena in priprava testne raztopine iz različnih vzorcev predstavljata najbolj kritično fazo analize. Ločbo velikega števila geometrijskih izomer likopena smo izvedli na koloni C30, z

and one form of PG were isolated using short monolithic columns (CIM® disks, Bia Separations d.o.o., Ljubljana, Slovenia). Both enzymes (pure PME and pure PG with preserved activity) were used in the year 2005 by the company Catchmabs (Wageningen) as targets for the iMab generation, and thereafter for the development of the method for the direct isolation of these enzymes from tomato extract by means of affinity chromatography.

- We investigated also what source of carotenoid lycopene are different commercial products on Slovenian market (tomato purees, ketchups, double concentrates, a dietary supplement formulated as tablets, etc). Extraction of lycopene and preparation of the test solutions was found to be the most critical phase of the analysis. The separation of a great number of geometrical isomers of lycopene was performed on the column C30 using a single component mobile phase, which is a big advantage of our method compared to the published methods. So we determined not only the total content of lycopene in different samples but also the content of isomers.
- In the frame of cooperation with the group from University of Helsinki (Faculty of Pharmacy, Finland) we finished the work about the TLC separation of catechins. With the partners from Palacky University (Faculty of Medicine, Institute of Medical Chemistry and Biochemistry, Olomuc, Czech Republic) we investigated biological and chemical variability of yacon (*Smalanthus sonchifolius*). Colleagues from the Institute for hop and brewing industry from Žalec, Slovenia, prepared us the first group of samples of roots of plants from Boraginaceae family containing bioactive naphtoquinones. Within the collaboration with researchers from Biotechnical Faculty (Department of Agronomy, Ljubljana, Slovenia), we performed some preliminary experiments with cuticular extracts of cabbage. Samples were taken from cabbages

enokomponentno mobilno fazo, kar je bistvena prednost v primerjavi z objavljenimi metodami. Tako nismo določili samo skupne vsebnosti likopena v različnih vzorcih, ampak tudi vsebnost izomer.

- S partnerji z University of Helsinki (Faculty of Pharmacy), Finska, smo dokončali delo o TLC ločbi katehinov. S partnerji s Palacky University (Faculty of Medicine, Institute of Medical Chemistry and Biochemistry), Olomuc, Češka, pa smo sodelovali pri raziskovanju biološke in kemijske variabilnosti jakuna (*Smalanthus sonchifolius*). Sodelavci z Inštituta za hmeljarstvo in pivovarstvo iz Žalca so nam pripravili prve vzorce korenin rastlin iz družine srbkolistnic, ki naj bi vsebovali zdravilne naftokinone. S sodelavci z Biotehniške fakultete (Oddelek za agronomijo) Univerze v Ljubljani smo naredili preliminarne poskuse z ekstrakcijo snovi s površin listov zelja. Zelje se je razlikovalo po naravni odpornosti proti določenim škodljivim žuželkam. Prvi rezultati so pokazali, da med odporno in neodporno vrsto zelja obstajajo razlike na molekularnem nivoju.
- V okviru sodelovanja s skupino z University of Belgrade (Faculty of Pharmacy), Srbija in Črna gora, smo razvili HPLC metodo za določanje fluorokinolonskega antibiotika norfloksacina v tabletah in metodo za določanje nečistot oziroma razgradnih

that differed in their natural resistance against chosen harmful insects. First analytical results showed that differences between resistant and unresistant species exist on molecular level.

- Within the cooperation with the group from University of Belgrade (Faculty of Pharmacy), Belgrade, Serbia and Montenegro, we developed a method for the determination of fluoroquinolone antibiotic norfloxacin in tablets and a method for the determination of impurities and degradation products in tablets with norfloxacin as the active ingredient. We studied conditions for TLC densitometric determination of norfloxacin by means of UV absorption or natural fluorescence of the compound.
- Within the cooperation with the group from Medical Centre Ljubljana, Slovenia, we investigated the influence of enteral nutrition (with different dietary supplements with specific action on the digestive organs) on intestinal permeability and healing in multiple injured patients. Intestinal permeability was evaluated by determination of lactulose and mannitol in 43 urine samples. The ratio of lactulose/mannitol excretion in urine after their administration is of great importance for evaluation of malabsorption and intestinal permeability disruption in some diseases.



SLIKA 2

Prvi prehrambeni izdelki z dodatkom vodotopnega Q10 izdelani po licenci Kemijskega inštituta

FIGURE 2

The first group of food products with water soluble Q10 prepared according to the license of National Institute of Chemistry

produktov v tabletah z norfloksacinom kot učinkovino. Proučevali smo tudi pogoje za TLC denzitometrično določanje norfloksacina preko UV absorpcije ali naravne fluorescence te spojine.

- V sodelovanju s skupino s Kliničnega centra iz Ljubljane smo raziskovali vpliv različnih prehranskih dodatkov (s specifičnim delovanjem na prebavila) na prepustnost črevesne stene in na potek zdravljenja politraumatiziranih poškodovancev. V ta namen smo s TLC analizo metodo določili laktulozo in manitol v 43 vzorcih urina. Na osnovi razmerja med laktulozo in manitolom smo ugotavljali prepustnost črevesne stene.

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; Fructal d.d., Ajdovščina; Pivovarna Union d.d., Ljubljana; BIA Separations d.o.o., Ljubljana in institucijami: Klinični center Ljubljana; Veterinarska fakulteta, Univerza v Ljubljani; Veterinarska klinika, Ljubljana; Zavod za zdravstveno varstvo Maribor; Biotehnična fakulteta, Univerza v Ljubljani; Inštitut za varovanje zdravja, Ljubljana itd.

MEDNARODNO SODELOVANJE

- Evropski projekt CRAFT: "Development of new food additives extracted from the solid residue of tomato processing industry for the application in functional food" (5. okvirni program EU, TOM)
- Bilateralni projekt Slovenija – Srbija in Črna gora z University of Belgrade, Faculty of Pharmacy (Beograd, Srbija in Črna gora): "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

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 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; Institut for Public Health Maribor, Slovenia...).

INTERNATIONAL COLLABORATION

European project:

- CRAFT: "Development of new food additives extracted from the solid residue of tomato processing industry for the application in functional food" (5th Framework Programme, TOM)

Bilateral project:

- Slovenia – Serbia and Montenegro: "Chromatographic methods in analysis of pharmacologically active compounds, investigation of QSPR and QSAR" with University of Belgrade, Faculty of Pharmacy (Belgrade, Serbia and Montenegro); principal researchers: I. Vovk and D. Agbaba

IMPORTANT INSTRUMENTS AND OTHER EQUIPMENT

Laboratory for food chemistry is equipped with HPLC systems with different type 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.

EDUCATION AND IMPORTANT VISITS

Seven students from different faculties from University of Ljubljana, Slovenia, finished their

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 je tudi 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 2005 je v laboratoriju sedem študentov z različnih fakultet Univerze v Ljubljani opravilo praktični del diplome in tudi diplomiralo. Dve mladi raziskovalki, B. Lapornik in M. Stražičar sta doktorirali in se zaposlili v industriji, prva v Krki d.d., Novo mesto; druga pa v slovenskem predstavništvu podjetja Merck & Co., Inc.

V letu 2005 sta laboratorij L06 obiskala:

- Prof. Gian Paolo Littarru, University of Ancona, Italija, predsednik mednarodnega združenja KoencimQ10
- Dr. Jose. L. Quiles, University of Granada, Španija

Gostovanja tujih raziskovalcev:

- Prof. dr. Danica Agbaba in prof. dr. Gordana Popović: Faculty of Pharmacy, University of Belgrade, Beograd, Srbija in Črna gora

practical work in our Laboratory and took diplomas. Two young researchers B. Lapornik and M. Stražičar took their degree of doctors in the year 2005. Brigita is now employed in pharmaceutical factory Krka d.d., Novo mesto, Slovenia and Monika in Slovenian representative of firma Merck & Co., Inc.

In the year 2005 two well-known representatives of International CoenzymeQ10 Association visited our laboratory:

- Prof. Gian Paolo Littarru, University of Ancona, Italy, the President of International CoenzymeQ10 Association, and
- Dr. Jose L. Quiles, University of Granada, Spain

Research visits:

- Prof. Dr. Danica Agbaba and Prof. Dr. Gordana Popović (Faculty of Pharmacy, University of Belgrade, Belgrade, Serbia and Montenegro)

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 (od / since 1. 11. 2005)

Dr. Andrej Kržan

Doc. dr. Matjaž Kunaver

Dr. Ida Mav Golež

Dr. Ema Žagar

**MLADA RAZISKOVALCA /
YOUNG RESEARCHERS**

Blaž Brulc (od / since 1. 11. 2005)

Maja Gričar

TEHNIČNO OSEBJE / TECHNICAL STAFF

Miran Lavrič

Mira Mikuž (do / until 31. 8. 2005)

Polona Prosen

Mirjana Širca



PODROČJA DEJAVNOSTI

Raziskave so potekale v okviru raziskovalnega programa P2-0145-0104 (Polimeri s posebnimi lastnostmi), enega temeljnega in štirih aplikativnih projektov, evropske mreže odličnosti, petih bilateralnih projektov in projektov za naročnike; dva evropska projekta iz 5. OP sta se po podaljšanju iz leta 2004 zaključila.

Področja dejavnosti L07 so:

- Visoko razvejeni polimeri
- Biorazgradljivi polimeri
- Polimeri iz obnovljivih surovin
- Delno prepletene polimerne mreže iz funkcionaliziranih poliuretanskih in poli-metakrilatnih predpolimerov
- Prevodne kompozitne polimerne membrane iz temperaturno obstojnih polimerov s polarnimi nosilci naboja in prevodni polimeri na osnovi substituiranih polianilinov
- Modificirani nanodelci, polimerni nanokompoziti
- Recikliranje sintetičnih polimerov
- Lastnosti polimerov in polimernih materialov

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:

- Hyperbranched polymers
- Biodegradable polymers
- Polymers from renewable resources
- Semi-interpenetrating polymer networks based on functionalized polyurethane and polymethacrylate prepolymers
- Conductive composite polymer membranes made of thermally resistant polymers with polar charge carriers and conductive polymers based on substituted polyanilines
- Modified nanoparticles, polymer-based nanocomposites
- Recycling of synthetic polymers
- Properties of polymers and polymeric materials

- 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
- Applied and development research, especially for industry of binders, thermoplastics, and recycling
- Analysis and characterization of commercial polymers by spectroscopic (FTIR, NMR), chromatographic (GC, GC-MS, IGC, SEC, SEC-MALS) and thermal techniques (DSC)

BIBLIOGRAFIJA

- 16 izvirnih znanstvenih člankov
- 2 strokovna članka
- 2 polemiki, diskusijska prispevka
- 3 drugi članki ali sestavki
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanje)
- 10 objavljenih znanstvenih prispevkov na konferencah
- 2 objavljena strokovna prispevka na konferencah
- 27 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 2 objavljena povzetka strokovnih prispevkov na konferencah
- 2 patenta
- 8 predavanj na tujih univerzah
- 2 prispevka na konferencah brez natisa
- 2 končni poročili o rezultatih raziskav
- 3 diplome
- 1 magisterij
- 1 doktorat
- 5 uredništvev revij

GLAVNI DOSEŽKI V LETU 2005

- Raziskali smo vpliv staranja visoko razvejenega komercialnega alifatskega poliestra pri različnih temperaturah na njegove strukturne, reološke in termične lastnosti. Pri visokorazvejenih polimerih, ki jih v splošnem uvrščamo med amorfne polimere, pri določenih pogojih lahko nastane mikrostruktura različne stopnje urejenosti, ki močno vpliva na njihove lastnosti. Termično in reološko obnašanje poliestra je posledica urejanja strukture preko H-vezi med linearnimi sekvencami, ki so v visokorazvejanem poliesteru prisotne kot nepravilnosti v strukturi.

BIBLIOGRAPHY

- 16 Original Scientific Articles
- 2 Professional Articles
- 2 Polemics, Discussions
- 3 Other Articles or Component Parts
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 10 Published Scientific Conference Contributions
- 2 Published Professional Conference Contributions
- 27 Published Scientific Conference Contribution Abstracts
- 2 Published Professional Conference Contribution Abstracts
- 2 Patents
- 8 Invited Lectures at Foreign Universities
- 2 Unpublished Conference Contributions
- 2 Final Research Reports
- 3 Undergraduate Theses
- 1 Master's Thesis
- 1 Doctoral Dissertation
- 5 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2005

- We investigated the effects of annealing the commercial hyperbranched aliphatic polyester at different temperatures on its structural, rheological, and thermal properties. Hyperbranched polymers, generally considered as amorphous materials, can form in some instances microstructures of different ordering degrees, which influences their properties considerably. Polyester thermal and rheological behaviour is a consequence of structural ordering through formation of H-bonds between linear sequences, which are present in the hyperbranched structure as the defects.

Urejenost je največja pri nizkomolekularni frakciji poliestra, ki ima odprto strukturo in najnižjo stopnjo razvejanja.

- Raziskave molekulske dinamike linearnega in visoko razvejenega poliuretana ter njenih mešanic z dielektrično spektroskopijo in dinamično mehansko analizo so pokazale, da pri molekulske dinamiki mešanic prevladuje prispevek linearnega poliuretana, medtem ko razvejeni poliuretan vpliva le na primarno relaksacijo, ki je povezana s temperaturo steklastega prehoda pri višji temperaturi.
- Biorazgradljivim amfifilnim kopolimerom poli(sukcinimid-ko-laktid), PSL, z različno kemijsko sestavo smo določili relativna in absolutna povprečja molskih mas ter njihovo porazdelitev. Po dostopnih literarnih podatkih je to prva analiza PSL kopolimerov z absolutno metodo SEC-MALS. Velike razlike med absolutnimi in relativnimi povprečji molskih mas smo pojasnili z razlikami v kemijski sestavi kopolimerov in PS standardov ter z bolj kompaktno konformacijo PSL kopolimerov v topilu zaradi razvejanja in zaradi intramolekularnih hidrofobnih interakcij med laktidnimi enotami.
- Na področju polimerov iz obnovljivih surovin smo nadaljevali raziskave utekočinjanja lesa in njegove uporabe za sintezo nasičenih in nenasičenih poliestrov. Les nativnih listavcev smo utekočinili z različnimi glikoli z uporabo kislinskega katalizatorja, pri čemer se je utekočinilo do 95% lesa. Še boljši izkoristek smo dosegli z uporabo mikrovalov, kot vira termične energije. Utekočinjen les smo uporabili za sintezo poliestrov z vključenimi razgradnimi produkti lesnih komponent. Nasičen poliester smo uporabili za sintezo trde poliuretanske pene. Rezultate raziskav smo patentirali v treh slovenskih patentih.
- Sklenili smo raziskave molekulske dinamike delno prepletenih polimernih mrež in mešanic iz funkcionaliziranih poliuretanov in poli-metakrilatov z elektronsko spinsko resonanco (metoda spinskega označevalca) in potrdili

The ordering of the structure is highest in the case of low molar mass fraction of polyester, which has an open structure and the lowest degree of branching.

- The molecular dynamics of blends of linear and hyperbranched polyurethanes (HB PU) is dominated by the relaxation phenomena of the linear component, which prevails over the secondary relaxations of the HB PU. The HB component influences the molecular dynamics of blends only in the case of the α -process connected with the high-temperature T_g , which appears between T_g temperatures characteristic of the pure components.
- We determined relative and absolute molar mass averages (MMA) and distributions (MMD) of the synthesized biodegradable amphiphilic copolymers poly(succinimide-co-lactide)s, PSL, with different chemical composition. According to the literature this is the first analysis of PSL copolymers by using the absolute technique SEC-MALS (size exclusion chromatography coupled to multi-angle light scattering photometer). Large differences between relative and absolute MMA were ascribed to the difference in copolymer and polystyrene composition and to a very compact conformation of PSL in solution due to branching and intramolecular hydrophobic interactions.
- In the use of renewable resources for polymer production we continued with research on wood liquefaction and its use in the synthesis of saturated and unsaturated polyesters. Native hardwoods were liquefied with the use of various glycols and organic acid catalyst. Liquefaction of up to 95% was achieved. By using microwaves as the heating source we have achieved almost 100% liquefaction. Liquefied wood was then used as the feedstock for synthesis of polyesters that contained incorporated degradation products of wood components. Saturated polyesters were used for synthesis of hard polyurethane foams. Results are protected by three slovenian patent rights.

- vpliv interakcij med komplementarnimi funkcionalnimi skupinami na heterogenost segmentnega gibanja in na fazne prehode.
- Delo na ionsko prevodnih polimernih membranah smo nadaljevali s pripravo sklopa membrane in elektrod (angl. Membrane electrode assembly, MEA), s katerim smo preizkusili delovanje lastnih membran v testni postaji in določili njihove elektrokemijske lastnosti.
 - Po poliolnem postopku smo sintetizirali (nano)delce bakrovega (I) oksida, kovinskega bakra in srebra, cinkovega oksida in nanožičke Cu_2O v različnih diolih. Delci velikosti med 100 nm in 10 μm so bili večinoma aglomerirani, na površini pa je bilo adsorbirano topilo, ki hkrati ščiti delce pred oksidacijo in omogoča boljšo disperzibilnost delcev v organskih medijih.
 - Nanokompozite iz modificiranega montmorilonita (MMT) in PMMA smo pripravili v
- The molecular dynamics of semi-interpenetrating polymer networks and polymer mixtures based on functionalised polyurethanes and methacrylic copolymers was investigated by electron spin resonance – spin label method. The influence of polymer interactions imposed by complementary functional groups on motional heterogeneity and phase transitions was confirmed.
 - The research on ion-conducting polymer membranes was focused on the preparation of membrane-electrode assemblies (MEA) which were used to test the electrochemical characteristics of our own membranes in a fuel cell test station.
 - (Nano)particles of copper (I) oxide, metallic copper, silver, zinc oxide and nanowires of copper (I) oxide were synthesized by the polyol procedure in different diols. Particles with sizes between 100 nm and 10 μm were mostly agglomerated. Solvent (diol) was



SLIKA 1:
Dvopolžni ekstruder Teach-Line ZK 25T z vodno kopeljo in granulatorjem, Dr. Collin.

FIGURE 1:
Twin screw extruder Teach-Line ZK 25T with water bath and strand pelletizer, Dr. Collin.

talini z dvopolžnim ekstruderjem ali z enostopenjsko in situ polimerizacijo. Po postopku v talini so nastali interkalirani nanokompoziti z nekaj višjo temperaturo steklastega prehoda od PMMA, termična stabilnost pa je bila izboljšana šele pri temperaturah nad 300°C. Enostopenjska in situ polimerizacija je nov postopek priprave polimernih nanokompozitov, pri katerem reakcija polimerizacije poteka v topilu etanol/voda v prisotnosti kvarterne amonijeve soli, MMT in iniciatorja, po zaključeni reakciji pa polimer oborimo z vodo. Nastanejo interkalirani nanokompoziti, katerih termična stabilnost je bistveno izboljšana v primerjavi s PMMA. Razvili smo tudi postopek priprave oksidnih ali kovinskih PMMA nanokompozitov z redukcijo ali hidrolizo in situ med polimerizacijo metilmetakrilata v masi.

- Nanokompozite smo pripravili tudi iz komercialnih vzorcev modificiranega MMT in naravnega kavčuka. Ugotavljali smo vpliv časa mešanja na vrivanje elastomernih molekul med plasti MMT ter vpliv MMT na zamreževanje in reološke lastnosti gume. Prisotnost MMT v gumeni zmesi je povečala hitrost zamreževanja kavčuka. Nastali so interkalirani nanokompoziti.
- Za industrijskega partnerja smo na osnovi recikliranega polietilentereftalata sintetizirali serijo nenasičenih poliestrskih smol in poliestrskih smol kot dodatkov za preprečevanje skrčkov pri zamreženju nenasičenih poliestrskih smol. Dve formulaciji sta bili izbrani za pilotno sintezo.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Renault, Francija: protonsko prevodne visoko temperaturne membrane za gorivne celice (odg. nosilec iz L13)
- Razvojno tehnološki inštitut, Savatech d.o.o., Kranj: sodelovanje pri raziskovalnem programu in projektu na področju elastomernih nanokompozitov

adsorbed on the particle surface protecting them from oxidation as well as improving their dispersibility in organic media.

- Nanocomposites of modified montmorillonite (MMT) and poly(methyl methacrylate) (PMMA) were prepared by melt intercalation using twin-screw extruder or by one-step in situ polymerization. The nanocomposites prepared by melt intercalation exhibit only a slightly higher glass transition temperature (T_g) than pure PMMA, whereas the thermal stability was improved at temperatures above 300 °C. One step in situ polymerization is a novel process for the preparation of nanocomposites. The polymerization proceeds in an ethanol/water solvent mixture in the presence of a quaternary ammonium salt, MMT and an initiator. Intercalated PMMA nanocomposites were precipitated in water. Their thermal stability was greatly improved compared to PMMA synthesized under the same conditions. A new method was developed to prepare PMMA nanocomposites with metallic or metallic oxide nanoparticles by reduction or hydrolysis during the in situ bulk polymerization.
- We also prepared intercalated nanocomposites of natural rubber and commercial MMT. The influence of mixing time on intercalation of elastomeric molecules between the layers of MMT, and the influence of MMT on crosslinking and rheological properties were examined. The presence of MMT in rubber mixture increased crosslinking.
- In cooperation with our industrial partner we synthesized a series of unsaturated polyester resins and low-profile additives for polyester resins based on recycled polyethylene terephthalate. Two formulations were chosen for pilot synthesis testing.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Renault, France: Proton conductive high-temperature polymer membranes for fuel cells (principal investigator from L13)

- Fakulteta za strojništvo, Univerza v Ljubljani in Institut Jožef Stefan: sodelovanje pri raziskovalnem projektu na področju polimernih nanokompozitov
- Color d.d., Medvode: sodelovanje pri aplikativnem projektu na področju uporabe odpadnega polietilentereftalata
- KLI Logatec in Biotehniška fakulteta, Univerza v Ljubljani: sodelovanje pri aplikativnem projektu na področju sinteze veziv in razvoja novih premaznih sistemov z nizko vrednostjo HOS za lesno industrijo
- Fakulteta za farmacijo, Univerza v Ljubljani: sodelovanje pri aplikativnem projektu na področju inverzne plinske kromatografije
- Institut Jožef Stefan: sodelovanje pri aplikativnem projektu na področju uporabe visoko reaktivne plazme
- Termo d.d., Škofja Loka: industrijski projekt na področju izolacijskih materialov (Ministrstvo za gospodarstvo)
- PPG Industries, ZDA: raziskovalno-razvojno sodelovanje
- Tehnološka platforma Napredni materiali: sodelovanje pri organizaciji aktivnosti delovanja tehnološke platforme
- Za različne partnerje iz industrije (Julon d.d., Ljubljana; Kolektor d.o.o., Idrija; Plama-pur d.d., Podgrad; Proizvodnja kemičnih izdelkov TKK Srpenica d.d., Srpenica; Veplas d.d., Velenje; Tekstilna tovarna Okroglica d.d., Volčja Draga; Lek d.d., Ljubljana itd.) analiziramo polimerne materiale in rešujemo strokovne probleme
- Research & Technology Institute, Savatech d.d., Kranj, Slovenia: Elastomer-based nanocomposites (research program and project)
- Faculty of Mechanical Engineering, University of Ljubljana, Slovenia and Jožef Stefan Institute, Ljubljana, Slovenia: Polymer-based nanocomposites (applied project)
- Color d.d., Medvode, Slovenia: The application of waste polyethylene terephthalate (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)
- Faculty of Pharmacy, University of Ljubljana, Slovenia: Determination of surface properties by inverse gas chromatography (applied project)
- Jožef Stefan Institute Ljubljana, Slovenia: Highly reactive plasma (applied project)
- Termo d.d., Škofja Loka, Slovenia: research on insulation materials (industrial project)
- PPG Industries, USA: research&development collaboration
- Technological platform Advanced Materials: activities in connection to organization of the technological platform
- We analyse polymeric materials and solve professional problems for our industrial partners (Julon d.d., Ljubljana, Slovenia; Kolektor d.o.o., Idrija, Slovenia; Plama-pur d.d., Podgrad, Slovenia; TKK Srpenica d.d., Srpenica, Slovenia; Veplas d.d., Velenje, Slovenia; Tekstilna tovarna Okroglica d.d., Volčja Draga, Slovenia; Lek d.d., Ljubljana, Slovenia...)

MEDNARODNO SODELOVANJE

- Projekt, 5. OP EU, 2002 - 2004, podaljšanje do 2005: Dairy industry waste as source for sustainable polymeric material production, WHEYPOL
- Sodelovanje pri projektu 5. OP EU, 2001 - 2004, podaljšanje do 2005: Advanced PEM fuel cells, APOLLON (odg. nosilec iz L13)

INTERNATIONAL COLLABORATION

- 5. OP EU, 2002 - 2004, extension to 2005: Dairy industry waste as source for sustainable polymeric material production, WHEYPOL

- Mreža odličnosti, 6. OP EU, 2004 - 2008: Nanostructured and functional polymer-based materials and nanocomposites, NANOFUN-POLY
- Bilateralni projekti:
 - Italija (2003 - 2005), University of Pisa, Department of Chemistry and Industrial Chemistry: Okoljsko razgradljivi polimerni materiali in plastika v Sloveniji
 - Srbija in Črna gora (2004 - 2005), Tehnološko metalurški fakultet, Univerzitet u Beogradu: Biorazgradljivi polimeri
 - Velika Britanija (2005), University of Leeds: A synthesis and characterisation of polymers from renewable sources
 - Hrvaška (2005 - 2006), Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u
- Collaboration within 5. FP EU, 2001 - 2004, extension to 2005: Advanced PEM fuel cells, APOLLON (principal investigator from L13)
- Network of Excellence, 6. FP EU, 2004 - 2008: Nanostructured and functional polymer-based materials and nanocomposites, NANOFUN-POLY
- Bilateral projects:
 - Italy, 2003 - 2005 (University of Pisa, Department of Chemistry and Industrial Chemistry): Environmentally degradable polymeric materials and plastics in Slovenia
 - Serbia and Montenegro, 2004 - 2005 (Faculty of Technology and Metallurgy, University of Belgrade): Biodegradable polymers
 - United Kingdom, 2005 (University of Leeds):



SLIKA 2:
Stroj za injekcijsko vbrzganje Babyplast, Rambaldi+Co.

FIGURE 2:
Injection moulding machine Babyplast, Rambaldi+Co.

Zagreb: Polimerni nanokompozitni materiali na osnovi montmorillonita

- 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 1725X, 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 dvo-dimenzionalne kromatografije
- Tekočinski kromatograf z detektorjem na sipanje svetlobe (Hewlett Packard, Wyatt Technology Corporation) za meritve SEC-MALS
- Souporaba mikrovalovne pečice Milestone MLS 1200 Mega
- Souporaba velike inštitutske opreme (NMR, XRD, LC-MS, SEM)
- 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:

- Mojca Merhar (BIA Separations d.o.o., Ljubljana): doktorska disertacija Vpliv sestave reakcijske mešanice na strukturne lastnosti polimernih monolitnih kromatografskih nosilcev in primeri njihove uporabe, Fakulteta

A synthesis and characterisation of polymers from renewable sources

- Croatia, 2005 - 2006 (Faculty of Chemical Engineering and Technology, University of Zagreb): Polymeric nanocomposites based on montmorillonite
- 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 1725X, Perkin Elmer
- 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 large Institute's equipment (NMR, WAXS, 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

Mentorships:

- Mojca Merhar (BIA Separations d.o.o., Ljubljana, Slovenia), Doctoral dissertation: Influence of reaction mixture composition on

za kemijo in kemijsko tehnologijo, Univerza v Ljubljani

- Nada Verdel: magistrsko delo Raziskave kopolimerov asparaginske in mlečne kisline, Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani
- Peter Večko: diplomsko delo (VSŠ) Razklop lesa z uporabo mikrovalov, Biotehniška fakulteta, Univerza v Ljubljani
- Mihael Volk: diplomsko delo (VSŠ) Uporaba utekočinjenega lesa za sintezo alkidnih smol, Biotehniška fakulteta, Univerza v Ljubljani
- Janez Glasenčnik: diplomsko delo (VSŠ) Utekočinjen les kot sredstvo za izdelavo polimerov, Biotehniška fakulteta, Univerza v Ljubljani

Habilitacija:

- M. Žigon: izr. prof. za polimerno inženirstvo (Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani)

Obiski:

- E. Žagar se je izpopolnjevala na področju dvodimenzionalne kromatografije na Univerzi v Amsterdamu, Nizozemska (05. 02. - 19. 02. 2005)
- E. Žagar je v okviru Nanofun-poly mreže odličnosti je gostovala na Leibniz-Institut für Polymerforschung (IPF) v Dresdnu, Nemčija (07. 09. - 11. 09. 2005) in v tovarni Synpo v Pardubicah, Češka (12. 09. - 16. 09. 2005); namen gostovanja je bil razgovor o sodelovanju med partnerji Nanofun-poly mreže na področju karakterizacije visoko razvejenih polimerov
- V okviru bilateralnega sodelovanja so L07 obiskali (tedenski obiski): prof. dr. Jirí Vohlídal, Charles University, Praga, Češka, prof. dr. Ivanka Popović, Univerzitet u Beogradu, Srbija in Črna gora in prof. dr. Jim Guthrie, University of Leeds, Velika Britanija

DVOPOLŽNI LABORATORIJSKI EKSTRUDER IN STROJ ZA INJEKCIJSKO VBRIZGAVANJE

V letu 2004 smo v Laboratoriju za polimerno

the structural properties of monolith chromatographic supports and their applications, University of Ljubljana, Slovenia

- Nada Verdel, Master's thesis: Investigation of the copolymers of aspartic and lactic acids, University of Ljubljana, Slovenia
- Peter Večko, Diploma thesis (VSŠ) Wood liquifaction using microwaves, University of Ljubljana, Slovenia
- Mihael Volk, Diploma thesis (VSŠ) The use of liquid wood for the synthesis of alkyd resins, University of Ljubljana, Slovenia
- Janez Glasenčnik, Diploma thesis (VSŠ) Liquid wood as a raw material for polymer synthesis, University of Ljubljana, Slovenia

Habilitation:

- M. Žigon: Assoc. Prof. for Polymer Engineering (University of Ljubljana, Slovenia)

Visits:

- E. Žagar was a visiting researcher at the University of Amsterdam, Netherlands (05. 02. - 19. 02. 2005) in the field of two-dimensional chromatography
- E. Žagar was a guest at Leibniz-Institut für Polymerforschung (IPF), Dresden, Germany (07. 09. - 11. 09. 2005), and at Synpo, Ltd., Pardubice, Czech Republic (12. 09. - 16. 09. 2005) in the frame of collaboration with partners of the Network of Excellence Nanofun-poly: characterization of hyperbranched polymers
- Visitors in the frame of bilateral collaboration: Prof. Dr. Jirí Vohlídal, Charles University, Prague, Czech Republic; Prof. Dr. Ivanka Popović, University of Belgrade, Serbia and Montenegro and Prof. Dr. Jim Guthrie, University of Leeds, United Kingdom

TWIN-SCREW EXTRUDER AND INJECTION MOULDING MACHINE

In 2004 the research of the Laboratory for Polymer Chemistry and Technology was oriented towards the preparation of nanocomposites based on clay, nanowires and nanomagnets.

kemijo in tehnologijo začeli raziskovati pripravo nanokompozitov na osnovi gline, nanožičk in nanomagnetov. Vzpostavili smo povezave tako s slovenskimi kot tudi z evropskimi raziskovalci. Problem opremljenosti za pripravo in karakterizacijo nanokompozitov smo rešili v letu 2005, ko smo s pomočjo Ministrstva za visoko šolstvo, znanost in tehnologijo kupili dvopolžni laboratorijski ekstruder (Teach-Line ZK 25T, Dr. Collin GmbH) in stroj za injekcijsko vbrizgavanje (Babyplast, Rambaldi+Co.). Dvopolžni ekstruder je opremljen z vodno kopeljo za hlajenje in granuliranjem. Kapaciteta ekstruderja je do »3kg/h materiala, z njim pa lahko poleg nanokompozitov pripravljamo tudi klasične kompozite in polimerne mešanice. Z granuliranjem lahko kompozite ali mešanice pripravimo za nadaljnjo predelavo, ki jo omogoča stroj za injekcijsko vbrizgavanje, Babyplast. S primernim orodjem lahko pripravimo epruvete za določanje mehanskih lastnosti ali pa kakršenkoli izdelek do velikosti 9 cm³. Ker je Babyplast avtomatski miniaturni industrijski stroj, lahko pripravljamo tudi manjše ali večje serije izdelkov za industrijske partnerje.

We established connections with various research groups within Slovenia and Europe. The lack of equipment for preparation of nanocomposites and specimens for the testing of mechanical properties was solved in 2005. With the help of the Ministry of higher education, science and technology we purchased a twin-screw extruder Teach-Line ZK 25T (Dr. Collin GmbH) and injection moulding machine Babyplast (Rambaldi+Co.). The twin-screw extruder is equipped with a water bath and strand pelletizer. The capacity of the extruder is up to 3 kg/h, and it can also be used for the preparation of classical composites and polymer blends. The pelletizer enables us to prepare materials in a form, which can be directly used in further processing by the injection moulding machine. We use the latter to prepare test specimens for determination of mechanical properties, however, any other product of sizes up to 9 cm³ can be made. Since the Babyplast is a miniaturized industrial machine we are able to produce smaller or bigger series of products for our industrial partners.

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)

Mag. Urban Švajger (do / until 31. 7. 2005)

**MLADI RAZISKOVALEC /
YOUNG RESEARCHER**

Damjan Šterk

PRIPRAVNIK / TRAINEE

Jure Kokalj (od / from 15. 9. 2005)



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
- 2 objavljena povzetka znanstvenih prispevkov na konferencah
- 2 patentni prijavi
- 1 patent
- 1 prispevek na konferenci brez natisa
- 1 diploma
- 1 doktorat
- 1 uredništvo revije

GLAVNI DOSEŽKI V LETU 2005

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

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
- 2 Published Scientific Conference Contribution Abstracts
- 2 Patent Applications
- 1 Patent
- 1 Unpublished Conference Contribution
- 1 Undergraduate Thesis
- 1 Doctoral Dissertation
- 1 Journal Editorship

IMPORTANT ACHIEVEMENTS IN 2005

- Preparation of new chiral phosphane ligands and their Rh-complexes which showed high enantioselectivity and activity in asymmetric hydrogenation of functionalized C=C bonds

- Asimetrično hidrogeniranje s prenosom vodika endocikličnih C=N vezi s kiralnimi amin-sulfamoilamidnimi Ru-katalizatorji razvitimi v našem laboratoriju, pri čemer so nastali kiralni ciklični amini v visokem enantiomernem presežku
- Sinteza novih poliaminskih derivatov za preprečevanje sepse
- Sinteza novih fluoriranih antibiotikov
- Asymmetric transfer hydrogenation of endocyclic C=N bonds to obtain chiral cyclic amines in high enantiomeric excesses with our laboratory developed chiral amine-sulfamoylamide Ru-catalysts
- Synthesis of novel polyamine derivatives for preventing sepsis
- Synthesis of new fluorinated antibiotics

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- 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 - 2005 (Univerza Louis Pasteur,

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- 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,



SLIKA 1:

Sistem za hidrogeniranje pri 1 atm H₂ v odsotnosti zraka

FIGURE 1:

System for hydrogenation at 1 atm of H₂ with exclusion of air

Strasbourg, Francija): Novi katalizatorji za asimetrično hidrogeniranje s prenosom vodika vezani na nosilec

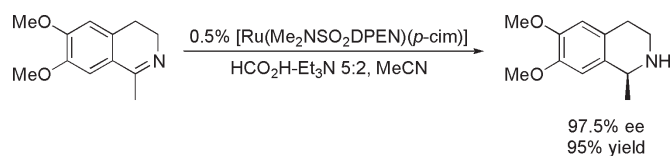
Strasbourg, France): New supported catalysts for asymmetric transfer hydrogenation

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

Primer asimetričnega hidrogeniranja s prenosom vodika 1-metil-6,7-dimetoksi-3,4-dihidroizokinolina z [Ru(Me₂NSO₂DPEN)(*p*-cimen)] katalizatorjem

SCHEME 1

An example of asymmetric transfer hydrogenation of 1-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline with [Ru(Me₂NSO₂DPEN)(*p*-cymene)] catalyst

L09

Laboratorij za anorgansko kemijo
in tehnologijo

Laboratory for Inorganic Chemistry
and Technology



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Dr. Alenka Ristić

Doc. dr. Nataša Zabukovec Logar

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**PODIPLOMSKI ŠTUDENT /
GRADUATE STUDENT**

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
- nuklearna magnetno resonančna spektroskopija
- rentgenska absorpcijska spektroskopija

BIBLIOGRAFIJA

- 8 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 2 druga članka ali sestavka
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanji)
- 1 objavljeni znanstveni prispevek na konferenci
- 19 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 3 predavanja na tujih univerzah
- 1 končno poročilo o rezultatih raziskav
- 1 doktorat
- 3 uredništva revij

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

- 8 Original Scientific Articles
- 1 Review Article
- 2 Other Articles or Component Parts
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 1 Published Scientific Conference Contribution
- 19 Published Scientific Conference Contribution Abstracts
- 3 Invited Lectures at Foreign Universities
- 1 Final Research Report
- 1 Doctoral Dissertation
- 3 Journal Editorships

GLAVNI DOSEŽKI V LETU 2005

Zeolitni materiali:

Naravni zeoliti se uporabljajo pri čiščenju odpadnih vod. V sodelovanju z Univerzo v Zagrebu, Hrvaška, smo jih preučevali z metodo rentgenske difrakcije na praškastih vzorcih.

Zeolit H-US-Y je eden od industrijsko najpomembnejših zeolitov. V sodelovanju z francoskim laboratorijem v okviru bilateralnega projekta PROTEUS smo z jedrsko magnetno resonanco v omenjenem zeolitu proučevali vlogo izven-ogrodnih aluminijevih kationov pri nevtralizaciji negativno nabitega zeolitnega ogrodja. V ta namen smo uporabili metodo za opazovanje sklopitev med bližnjimi aluminijevimi jedri, ki smo jo nedavno razvili v našem laboratoriju.

S kovinami modificirani mikroporozni aluminofosfati in kovinski fosfati so zaradi njihovih raznolikih ogrodnih struktur uporabni kot adsorbenti in katalizatorji. S hidrotermalno kristalizacijo smo sintetizirali nov s kromom modificiran aluminofosfat in dva nova cinkofosfata. Z metodo rentgenske praškove difrakcije in rentgenske difrakcije na monokristalih smo določili strukture novih produktov.

Mezoporozni materiali:

S prehodnimi kovinami modificirane zeolitne materiale (velikost por od 0.5 do 2 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, narave vgrajene kovine in njenega mesta vgradnje v ogrodje. Uporaba zeolitnih materialov pa je omejena, ko sodelujejo v reakciji molekule večjih kinetičnih premerov. Za takšne reakcije je bolj primerna uporaba mezoporoznih materialov z velikostjo por od 2 do 10 nm. Naše raziskave so bile v letu 2005 usmerjene v pripravo in strukturno karakterizacijo mezoporoznih aluminofosfatov in silikatov. Sintetizirali smo z

IMPORTANT ACHIEVEMENTS IN 2005

Zeolitic materials:

Natural zeolites used for wastewater treatments were investigated in collaboration with the University of Zagreb by X-ray powder diffraction structural studies.

H-US-Y zeolite is one of the most important zeolites used in industry. We investigated its zeolitic structure by using nuclear magnetic resonance (NMR) in collaboration with French laboratory in the frame of bilateral PROTEUS project. With homonuclear correlation experiment that was recently developed in our laboratory it was possible to elucidate the charge-compensating role of extra framework aluminium cations within zeolite framework.

Microporous metal-modified aluminophosphates and zincophosphates are used as adsorbents and catalysts due to their open-framework structures. Novel aluminophosphate modified by chromium and two new zincophosphates were hydrothermally synthesised. Single-crystal and X-ray powder diffraction methods were used for structure determinations of these new products.

Mesoporous materials:

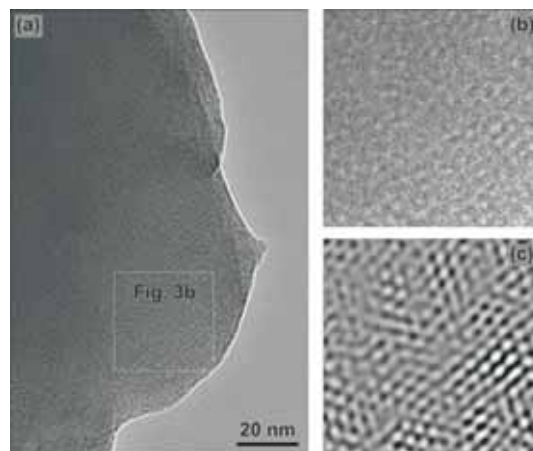
Transition-metal modified zeolitic materials with pore openings from 0.5 to 2 nm are widely used as heterogeneous catalysts in oxidation reactions. These catalysts possess remarkable catalytic activity due to transition-metal centres that are isolated within the zeolitic framework. Catalytic properties of these materials depend on structure type, location and on nature of incorporated metal. Pore size limitations of zeolitic catalysts can be overcome by using mesoporous aluminophosphates and silicates with pore openings from 2 to 10 nm when bulkier reactants have to be processed. We investigated the preparation and structure of mesoporous aluminophosphates and silicates. Manganese- and iron-modified mesoporous aluminophosphates (MnHMA and FeHMA) and manganese-modified mesoporous silicate (MnMCM-41) were synthesised. Mesoporous

manganom in železom modificirana mezoporožna aluminofosfata MnHMA in FeHMA ter z manganom modificiran mezoporožen silikat MnMCM-41. Mezoporožno strukturo smo raziskali z rentgensko difrakcijo (XRD) in presevnim mikroskopom visoke ločljivosti (HRTEM). Lokalno okolico mangana in železa smo določili z rentgensko absorpcijsko spektroskopijo (EXAFS, XANES), jedrsko magnetno resonanco (NMR), elektronsko paramagnetno resonanco (EPR) ter Mössbauerjevo spektroskopijo. Rezultati strukturne karakterizacije kažejo na termično stabilne mezoporožne materiale s katalitskimi lastnostmi zaradi vgrajenega mangana in železa v mezoporožno ogrodje. Nadaljnje raziskave produktov bodo potekale v sklopu sodelovanja z drugimi laboratoriji v okviru EU projekta INSIDE PORES.

structure was confirmed by X-ray powder diffraction (XRD) and high resolution transmission microscopy (HRTEM). X-ray absorption spectroscopy (XANES, EXAFS), nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) and Mössbauer spectroscopy revealed the local structure of manganese or iron. The characterisation results showed that stable mesoporous materials with catalytic properties were prepared. Further research on prepared products will include the collaboration with other laboratories within the frame of EU project INSIDE PORES.

Cement research:

The research with collaboration with Salanit Anhovo d.d., Deskle, Slovenia, resulted in the completion of the study on the influences of variously soluble carbonates on overall hydration and final phase development and compo-



SLIKA 1:

(a) HRTEM (Presevna Elektronska Mikroskopija Visoke Ločljivosti) fotografija delca mezoporožnega aluminofosfata. (b) Povečava izreza iz Slike (a) prikazuje domene s heksagonalno ureditvijo kanalov, ki pa so slabo vidne. (c) FFT filtrirana slika tega izreza razkrije vzorec s heksagonalno ureditvijo kanalov, ki je na več mestih prekinjen z dislokacijami, ki so delno posledica izpostavljanju močnega elektronskega toka na vzorcu.

FIGURE 1:

(a) HRTEM (High Resolution Transmission Electron Microscopy) image of the mesoporous aluminophosphate particle. (b) A close-up of the detail from the raw image in Fig. 3 (a) shows faint hexagonal features in some visible in some parts of the image. (c) FFT filtered image of this detail clearly reveals a close-packed hexagonal pattern disrupted with several dislocations and stacking faults, which have been partly induced by a relatively strong electron irradiation.

Cement:

V sklopu raziskav za SALONIT Anhovo smo zaključili raziskave vplivov različno topnih karbonatov na hidratacijo ter nastanek hidratiziranih faz v portland cementu. Topnostni parametri karbonatov vplivajo na nastanek specifičnih faz, čas hidratacije pa na končno fazno sestavo hidratiziranega cementa.

Sintetizirali smo čist tetrakalcijev monokarboaluminat 11-hidrat, ki se pojavlja v hidratiziranih cementih z apnencem, in ga okarakterizirali s termično analizo, praškovno rentgensko difrakcijo ter FTIR spektroskopijo.

Strukturna analiza drugih materialov:

Z jedrsko magnetno resonanco smo proučevali tudi z biološkega stališča zelo zanimive myo-inositol heksafosfatne spojine. Te spojine igrajo pomembno vlogo v prehrani, pri zdravju in tudi na področju konzervatorstva. Posebej zanimivo je delovanje fitatne kisline kot antioksidanta, ki z veliko afiniteto veže nase železo. S spektroskopijo fosforjevih jeder smo dobili vpogled v tvorbo vezi med atomi železa, kisika in fosforja in v lokalno strukturo v amorfni paramagnetni železovih fitatih.

Jedrsko magnetno resonanco smo uporabljali tudi za študij ionskih tekočin in karakterizacijo trdnih farmacevtskih vzorcev industrijskih partnerjev.

Vzporedno smo ves čas razvijali NMR metode za študij strukture anorganskih materialov.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Salonit Anhovo d.d., Deskle: raziskave in razvoj cementov z apnencem in mineralnimi dodatki
- Lek d.d., Ljubljana: rentgenska praškovna analiza in določanje specifične površine
- 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), koordinator:

sition in portland cement. Carbonate solubility parameters were shown to influence the formation of hydrated phases to various extents and hydration time dependencies were assessed.

Tetracalcium monocarboaluminate 11-hydrate, the compound that appears in hydrated limestone-containing portland cement, was synthesised and characterised by thermal analysis, X-ray powder diffraction and FTIR spectroscopy.

Structural analysis of other materials:

Application of broadline phosphorus NMR spectroscopy was extended to biologically relevant myo-inositol hexaphosphate (phytate) compounds. These compounds play an important role in nutrition, health and conservation sciences. Especially remarkable is an antioxidant property of the phytic acid, which derives from the high binding affinity of this acid for iron. Broadline phosphorus NMR provided insight into formation of bonds between phosphorus, oxygen, and iron atoms and offered a picture of a short-range structure within amorphous paramagnetic iron-phytates.

Several solid-state NMR measurements were performed also on samples of ionic liquids and on pharmaceutical samples from industrial partners.

In parallel, the methodology for structural description of inorganic materials was being developed.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Salonit Anhovo d.d., Deskle, Slovenia; Investigations and development of cements with limestone and mineral additives
- Lek d.d., Ljubljana, Slovenia: X-ray powder diffraction analyses and determination of specific surface areas
- Krka d.d., Novo mesto, Slovenia: X-ray powder diffraction analyses and determination of specific surface areas

- National Center for Scientific Research "Demokritos", Atene, Grčija
- Evropski sklad za regionalni razvoj (ESRR), Center odličnosti "Nanoznanosti in nanotehnologije" (2004 - 2006)
 - ESRR, 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, France
 - Slovensko - francoski bilateralni projekt, PROTEUS (2004 - 2005), Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija
 - Slovensko - angleški bilateralni projekt, PARTNERSHIP IN SCIENCE (2005), UMIST, Manchester, Velika Britanija
 - Slovensko - srbski bilateralni projekt (2004 - 2005), Tehnološko-metalurška fakulteta, Beograd, Srbija in Črna gora
 - Slovensko - hrvaški bilateralni projekt (2005 - 2006), Institut Ruđer Bošković, Zagreb, Hrvaška
 - Projekt z Univerzo v Manchestru v okviru sporazuma o znanstvenem sodelovanju med SAZU in The Royal Society, London, Velika Britanija

POMEMBNI INSTRUMENTI IN OPREMA

- Rentgenski praškovni difraktometer Siemens D 5000 (sevanje $\text{CuK}\alpha$ 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 $\text{CuK}\alpha$ z $\lambda = 1.5406\text{\AA}$) za snemanje praškovnih posnetkov v štirih različnih konfiguracijah: (1) α_1 z Johannsonovim monokromatorjem za vzorce

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 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 – Great Britain bilateral project, PARTNERSHIP IN SCIENCE (2005), UMIST, Manchester, Great Britain
- Slovenia - Serbia bilateral project (2004 - 2005), Faculty of Technology and Metallurgy, University of Belgrade, Serbia and Montenegro
- Slovenia - Croatia bilateral project (2005 - 2006), Rudjer Boskovic Institute, Zagreb, Croatia
- Project with University of Manchester within the frame of an agreement for scientific cooperation between Slovenian Academy of Sciences and Arts (SAZU) and The Royal Society, London, Great Britain

MAJOR EQUIPMENT

- X-ray powder diffractometer Siemens D 5000 (radiation wavelength $\text{CuK}\alpha = 1.5406\text{\AA}$) 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

- z ravno površino, (2) kapilarna transmisija s 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
- 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
- X-ray powder diffractometer PANalytical X'Pert PRO (radiation wavelength $\text{CuK}\alpha = 1.5406\text{\AA}$) for measurements of powder patterns on four different configuration: (1) alpha1 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 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 room temperature to 1500°C)
- Microtrac S3500 Particle Size Analyzer, wet or dry samples; the range of measurement



SLIKA 2:

Pridobitev laboratorija: Rentgenski praškovni difraktometer X'PertPRO MPD z visoko ločljivostjo.

FIGURE 2:

New instrument in the laboratory: X-ray powder high resolution diffractometer X'PertPRO MPD.

- Autopycnometer (Micromeritics Instrument Co.) aparatura za samodejno določevanje gostote materialov s helijem
- Centrifuga Hettich, Rotanta 460 R hlajena (temperaturno območje od -20°C do $+40^{\circ}\text{C}$). Hitrost obratov od 500 do 9.500min^{-1}
- Ultra Turrax disperzer T25 (IKA)
- Mikrovalovna peč MLS-1200 MEGA (Milestone)
- Mikrovalovna peč ETHOS (Milestone)
- Kalcinacijske peči: dve cevni (segrevanje do 1000°C , hitrost segrevanja $1.5\text{-}2^{\circ}\text{C}/\text{min}$) in ena komorna (segrevanje do 1200°C , hitrost segrevanja $3^{\circ}\text{C}/\text{min}$)

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Izobraževanje:

- Alenka Ristić je doktorirala 9. 6. 2005: »Sinteza molekularskih sit z železoaluminofosfatnim ogrodjem«, mentor: V. Kaučič
- Alen Kljajić je 29. 11. 2005 prejel Prešernovo nagrado Univerze v Ljubljani za raziskovalno nalogo z naslovom »Novi mezoporozni materiali na silikatni osnovi«, mentor: V. Kaučič

Obiski tujih raziskovalcev:

- dr. Frederic Thibault-Starzyk, Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija
- prof. Francis Taulelle, Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, Francija
- prof. Nevenka Rajić, Tehnološko-metalurška fakulteta, Univerza v Beogradu, Srbija in Črna gora
- Sanja Šajić, Tehnološko-metalurška fakulteta, Univerza v Beogradu, Srbija in Črna gora
- Nicolas Malicki, Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija
- mag. Karmen Margeta, Fakultet kemijskog inženjerstva i tehnologije, Sveučiliste Zagreb, Hrvaška

for wet samples is from $0.02\ \mu\text{m}$ to $1400\ \mu\text{m}$ ($2800\ \mu\text{m}$) and for dry samples from $0.25\ \mu\text{m}$ to $1400\ \mu\text{m}$

- 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 $+40^{\circ}\text{C}$). Speed control within a range of $500\text{-}9.500\text{min}^{-1}$
- Ultra Turrax disperzer T25 (IKA)
- Microwave oven MLS-1200 MEGA (Milestone)
- Microwave oven ETHOS (Milestone)
- Furnaces: two tubes (heating up to 1000°C , heating rate $1.5\text{-}2^{\circ}\text{C}/\text{min}$) and one chamber (heating up to 1200°C , heating rate $3^{\circ}\text{C}/\text{min}$)

EDUCATION AND IMPORTANT VISITS

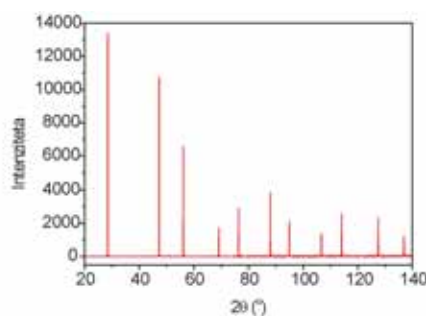
Education:

- Alenka Ristić ended her PhD thesis entitled »Synthesis of iron-aluminophosphate molecular sieves« on 9. 6. 2005, supervisor: V. Kaučič
- Alen Kljajić was awarded with University Prešeren Prize presented by the University of Ljubljana, Slovenia for undergraduate research project »Novel silicate-based mesoporous materials« on 29. 11. 2005, supervisor: V. Kaučič

Visits of foreign researchers:

- Dr. Frederic Thibault-Starzyk, Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, France
- Prof. Francis Taulelle, Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, France
- Prof. Nevenka Rajić, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia and Montenegro
- Nicolas Malicki, Laboratoire Catalyse & Spectrochimie, ISMRA-CNRS, Caen, France
- Sanja Šajić, Faculty of Technology and Met-

- dr. Cleo Kosanović, Institut Ruđer Bošković, Zagreb, Hrvatska
 - Sanja Bosnar, Institut Ruđer Bošković, Zagreb, Hrvatska
- Gostovanja:
- Saša Cecowski je gostovala v Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija (tri mesece)
 - Nataša Novak Tušar je gostovala v Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, Francija (1 teden)
 - Gregor Mali je gostoval na Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, France (2 tedna)
 - Nataša Zabukovec Logar je gostovala na UMIST, Manchester, Velika Britanija (1 teden)
 - Nataša Novak Tušar in Nataša Zabukovec Logar sta gostovali na Tehnološko-metalurški fakulteti, Univerza v Beogradu, Beograd, Srbija in Črna gora (1 teden)
 - Nataša Novak Tušar in Nataša Zabukovec Logar sta gostovali na Fakulteti za kemijsko inženirstvo in tehnologijo, Univerza v Zagrebu, Hrvatska
- allurgy, University of Belgrade, Belgrade, Serbia and Montenegro
 - Msc. Karmen Margeta, Faculty of chemical engineering and technology, University of Zagreb, Croatia
 - Dr. Cleo Kosanović, Ruđer Bošković Institute, Zagreb, Croatia
 - Sanja Bosnar, Ruđer Bošković Institute, Zagreb, Croatia
- Visits of foreign institutes:
- Saša Cecowski visited Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, France (3 months)
 - Nataša Novak Tušar visited Laboratory for Catalysis and Spectrochemistry, ISMRA-CNRS, Caen, France (1 week)
 - Gregor Mali visited Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, France (2 weeks)
 - Nataša Zabukovec Logar visited UMIST, Manchester, Great Britain (1 week)
 - Nataša Novak Tušar and Nataša Zabukovec Logar visited Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia and Montenegro (1 week)
 - Nataša Novak Tušar and Nataša Zabukovec Logar visited Faculty of Chemical Engineering and Technology, University of Zagreb, Croatia



SLIKA 3:

Difraktogram silicijevega standarda SRM640c posnet na rentgenskem praškovnem difraktometru X'PertPRO MPD z visoko ločljivostjo.

FIGURE 3:

X-ray powder patterns of silicon standard SRM640c measured on high resolution diffractometer X'PertPRO MPD.

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 Genorio

Mirjana Küzma

Dušan Strmčnik

TEHNIČNO OSEBJE / TECHNICAL STAFF

Gregor Kapun

Maja Mirič (polovični čas - od septembra /
part time – since september)

Milena Zorko



PODROČJA DEJAVNOSTI

Materiali za energijske in informacijske tehnologije:

- 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 ovojnica 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

- 11 izvirnih znanstvenih člankov
- 2 intervjuja

RESEARCH ACTIVITIES

Materials for energy and information technologies:

- 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

BIBLIOGRAPHY

- 11 Original Scientific Articles
- 2 Interviews

- | | | | |
|----|---|----|--|
| 1 | objavljeni znanstveni prispevek na konferenci (vabljeni predavanja) | 1 | Published Scientific Conference Contribution (Invited Lecture) |
| 5 | objavljenih znanstvenih prispevkov na konferencah | 5 | Published Scientific Conference Contributions |
| 15 | objavljenih povzетkov znanstvenih prispevkov na konferencah | 15 | Published Scientific Conference Contribution Abstracts |
| 1 | patentna prijava | 1 | Patent Application |
| 3 | končna poročila o rezultatih raziskav | 3 | Final Research Reports |
| 3 | elaborati, predštudije, študije | 3 | Treatises, Preliminary Studies, Studies |
| 2 | diplomi | 2 | Undergraduate Theses |

GLAVNI DOSEŽKI V LETU 2005

- Sinteza in karakterizacija novega materiala z bistveno večjo teoretično kapaciteto od doslej znanih materialov za pozitivne baterijske elektrode

V doslej znanih materialih za pozitivne elektrode v litijevih baterijah smo lahko za shranjevanje energije izkoristili največ 1 litij na molekulsko enoto materiala – čeprav je ta enota načeloma lahko vsebovala več kot 1 litij. S tem je bila specifična kapaciteta pozitivnih elektrod omejena na vrednosti med 150 in 170 mAh/g. V laboratoriju pa nam je uspelo sintetizirati povsem nov anorganski material, $\text{Li}_2\text{MnSiO}_4$, v katerem lahko za shranjevanje naboja teoretično izrabimo oba litija, kar pomeni, da znaša teoretična kapaciteta okoli 320 mAh/g. Žal v praksi zaenkrat te kapacitete nismo uspeli izkoristiti – pri praznjenju/polnjenju dobimo podobne vrednosti kapacitete kot v prej omenjenih klasičnih materialih. Vzrok so takorekoč izolatorske električne lastnosti silikatov (elektronska prevodnost za $\text{Li}_2\text{MnSiO}_4$ denimo znaša okoli 10^{-12} S/cm), kar upočasnjuje kinetiko do te mere, da v realnem času lahko izkoristimo le del razpoložljivega naboja. Glede na pretekle izkušnje s podobnimi izolatorskimi materiali pa obstaja realna možnost, da bomo z ustreznimi modifikacijami (zmanjševanjem povprečne velikosti delcev, dodajanjem prevodnih faz, morda celo z dopiranjem) precej izboljšali povprečno prevodnost elektrodnega kompozita ter posledično izkoristili znatno več kot 1 litij na molekulsko enoto

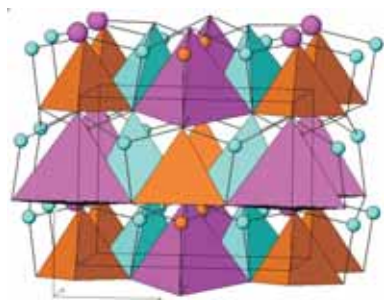
IMPORTANT ACHIEVEMENTS IN 2005

- Synthesis and characterization of a new material with a considerably higher theoretical capacity than in present materials for Li battery positive electrodes

In all existing materials for positive Li electrodes it is only possible to reversibly exchange up to 1 lithium per formula unit – even if the formula contains more than 1 lithium. This has limited the specific capacity of positive electrodes to values between 150 and 170 mAh/g. Recently we have synthesized a completely new inorganic compound, $\text{Li}_2\text{MnSiO}_4$, in which both lithium ions can in principle be exchanged so that the theoretical reversible capacity amounts as high as 320 mAh/g. Unfortunately, in practice we have not been able to exploit this huge capacity. In fact, upon material cycling we have obtained similar values of capacity as reported for other materials. The reason is the huge electrode polarization resulting from the insulating nature of silicates (for example, the electronic conductivity of $\text{Li}_2\text{MnSiO}_4$ is in the range of 10^{-12} S/cm) which limits the exploitation of available charge. However, based on our experience with other insulating active particles, we hope that in future we will be able to improve the average conductivity of electrode composites, either by particle size minimization, addition of conductive phases or even by heterogeneous doping. It can be claimed that eventual practical exploitation of more than 1 Li per formula unit will open a new chapter in search for high-energy density storage materials.

aktivnega materiala. S tem bi pridobili najboljši znani aktivni material za pozitivne elektrode v litijevih baterijah.

- Stabilizacija amorfni zdravil v vgradnjo učinkovine v mikroporozne anorganske gele
Priprava zdravilne učinkovine v amorfni obliki je pogosto zaželena, saj je v tem primeru njeno raztapljanje v organizmu praviloma hitrejše. Še pomembnejše je, da amorfne oblike zdravil niso patentno zaščitene. Največji problem amorfni oblik je ta, da niso stabilne in prehitro kristalizirajo. Tipičen primer takega zdravila je nifedipin, ki smo ga v študiji uporabili kot modelsko učinkovino. Na osnovi teoretičnih izračunov smo predpostavili, da bi lahko amorfno obliko nifedipina stabilizirali v porozni strukturi anorganskega gela. Računi so namreč pokazali, da v porah, ki so manjše od nekaj nanometrov, kristalizacija nifedipina zaradi prostorskih omejitev ne more poteci, zato se lahko izloči le v amorfni obliki. Ker bi bil nifedipin v mikroporah hkrati izoliran od okolice, bi bilo povsem možno, da bi s tem zelo upočasnili njegovo degradacijo. Poskusi so popolnoma potrdili teoretične predpostavke. Če smo namreč nifedipin vgradili v silikatno matrico s povprečnimi dimenzijami por okoli 2,5 nm, je nastala izključno amorfna oblika te učinkovine, stabilnost pa se je podaljšala od tipično nekaj dni na nekaj mesecev (morda še več - preskus stabilnosti je še vedno v teku).



SLIKA 1:
Struktura in elektrokemijska karakteristika novega baterijskega materiala: $\text{Li}_2\text{MnSiO}_4$

- Stabilization of amorphous drugs by incorporation of active substance into microporous inorganic gels

One of the advantages of amorphous drugs over their crystalline forms could be a faster dissolution in organism. For developers and pharmaceutical companies the amorphous forms of drugs are especially attractive as they are not patented. The most serious drawback of amorphous drugs is their instability leading to rapid and uncontrolled crystallization. A typical example is nifedipine which was used as a model substance in the present study. Based on theoretical calculations, we assumed that amorphous nifedipine could be stabilized within the porous structure of inorganic gels. Namely, as such pores are usually in the nanometre range, crystallization of nifedipine should not occur neither from liquid nor from the solid state - due to spatial constraint. Being embedded within the solid matrix and thus isolated from the surroundings, the drug, although amorphous, should be considerably stabilized. The experiments confirmed the predictions. When solidification of nifedipine took place within pores with an average size of ca. 2.5 nm, the resulting solid was completely amorphous and remained such over a period of several months instead of several days which is a typical stability period of the free amorphous nifedipine.

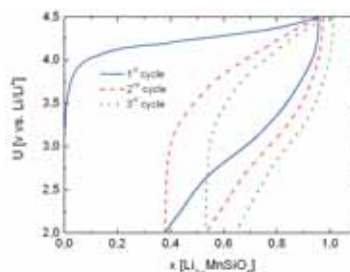


FIGURE 1:
Structure and electrochemical characteristics of a new battery material: $\text{Li}_2\text{MnSiO}_4$

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Iskra TELA d.d., 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 d.d., Litija; partner v Centru odličnosti Nanoznanosti in nanotehnologije, ESRR, ukrep 1.1. in 1.4
- Atotech Podnart d.d., Podnart; 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 EU

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 pri diplomah:

- Jože Moškon: Prevodne ogljikove prevleke na izbranih modelnih substratih; somentor: M. Gaberšček
- Aljaž Godec in Uroš Maver: Stabilizacija amorfnega nifedipina v kserogelu SiO₂; Prešernova nagrada, somentor: M. Bele

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Iskra TELA d.d., 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 d.d., Litija, Slovenia: partner in Nanosciences and Nanotechnologies Centre of Excellence
- Atotech Podnart d.d., Podnart, Slovenia: partner in Nanosciences and Nanotechnologies Centre of Excellence
- JUB d.d., Dol pri Ljubljani, Slovenia

INTERNATIONAL COLLABORATION

- ALISTORE, 6th EU Framework Network of Excellence

IMPORTANT INSTRUMENTS AND 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)

EDUCATION AND IMPORTANT VISITS

Mentors:

- Jože Moškon: «Conductive carbon coatings on selected model substrates»; diploma thesis; comentor: M. Gaberšček
- Aljaž Godec, Uroš Maver: «Stabilization of amorphous nifedipine in a SiO₂ xerogel», Prešern student award; comentor: M. Bele

Visits of foreign researchers:

- Emmanuel Baudrin, Laboratoire de Réactiv-

Obiski tujih raziskovalcev:

- Emmanuel Baudrin, Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie, Amiens, Francija
- Ion Matei, Max-Planck Institut fuer Festkoerperforschung, Stuttgart, Nemčija
- Rishi Raj, Department of Mechanical Engineering, Engineering Center - ECME 133, University of Colorado at Boulder, ZDA

Gostovanja:

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

Optimizacija delovanja baterij cink-zrak

Znanje, ki ga v laboratoriju pridobimo pri izvajanju programa in projektov, redno

ité et de Chimie des Solides, University of Picardie, Amiens, France

- Ion Matei, Max-Planck Institute, Stuttgart, Germany
- Rishi Raj, Department of Mechanical Engineering, Engineering Center - ECME 133, University of Colorado at Boulder, USA

Visits of foreign institutes:

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

Optimization of a zinc-air battery system

Knowledge that accumulates in the Laboratory during regular activities within the frames of national programme and other project is continuously transferred to Slovene industrial part-



SLIKA 2:

Dr. Marjan Bele predstavlja vrstični elektronski mikroskop na poljsko emisijo Karl Zeiss Supra 35 VP (novo pridobitev L10) dr. Janezu Potočniku, evropskemu komisarju za znanost in raziskave

FIGURE 2:

Dr. Marjan Bele is presenting a new Field-Emission Scanning Electron Microscope (Karl Zeiss Supra 35 VP) to Dr. Janez Potočnik, the European Commissioner for Science and Research

prenašamo v slovensko industrijo. V letih 2004 - 2005 smo izkušnje, ki smo jih pridobili pri raziskavah novih materialov za litijeve baterije, uporabili pri optimizaciji delovanja baterij cink-zrak, ki jih proizvaja podjetje Iskra TELA d.d., Šentvid pri Stični. Izkazalo se je namreč, da je tudi pri tem tipu baterij potrebno pripraviti pozitivno elektrodo z optimirano porozno arhitekturo, ki zagotavlja simultani dostop zraka, elektronov in ionov do čim večjega dela površine elektrode. S tem maksimiramo površinsko gostoto katalitskih mest za elektrodne reakcije, kar je ključno za delovanje baterije cink-zrak pri visokih tokovnih gostotah. Izboljšano delovanje baterij cink-zrak je Iskra TELA omogočilo sklenitev nove pogodbe, na osnovi katere je to podjetje postalo eden od vodilnih proizvajalcev specialnih baterij cink-zrak v Evropi.

ners. In the period of 2004 - 2005 we used the experience gained during the research of advanced lithium batteries in optimization of a zinc-air battery system produced by the national battery producer Iskra TELA d.d., Šentvid pri Stični, Slovenia. Like the electrodes in lithium batteries, the zinc-air battery also requires a carefully designed system of pores in order to provide a simultaneous access of air, electrons and ions to the electrocatalytic sites where the electrochemical reactions take place. Optimization of pore size and distribution, together with other improvements, lead to a successful maximization of current density and total capacity delivered by the zinc air battery. Based on these improvements, Iskra TELA has signed new contracts which launched this company among the most important European producers of zinc-air batteries for special applications.

L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation



VODJA / HEAD

Prof. dr. Radovan Komel

RAZISKOVALCI / RESEARCHERS

Dr. Aleksandra Comino
Dr. Marija Anžur Lasnik (LEK)
Dr. Apolonija Bedina Zavec
Maja Capuder
Menči Drole (LEK)
Dr. Irena Fonda
Dr. Vladimira Gaberc Porekar
Gorazd Hribar
Mag. Simona Jevševar (LEK)
Mag. Branka Korošec
Dr. Nada Kraševc
Dr. Ana Lenassi Zupan
Dr. Viktor Menart (KI / LEK)
Barbara Podobnik (LEK)

Dr. Marjetka Podobnik
Mag. Tatjana Preradov

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

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Maja Kenig (LEK)
Mateja Kusterle (LEK)
Ljerka Lah
Mateja Novak Štagoj
Špela Peternel
Matjaž Vogelsang

TEHNIČNO OSEBJE / TECHNICAL STAFF

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

GOSTUJOČI RAZISKOVALEC / VISITING SCIENTIST

Vanja Smilović



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" (L4-6171), "Steroidna 11beta-hidroksilaza iz nitaste glive *Cochliobolus lunatus*" (L4-4353) in "Strukturne raziskave inozitol-polifosfatnih kinaz" (J4-6463).

Raziskovalni program sestavljajo naslednja področja:

- Preučevanje metod za pridobivanje rekombinantnih citokinov
- 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.

Metodološki pristopi za izvajanje programa so:

- Gensko oziroma proteinsko inženirstvo:

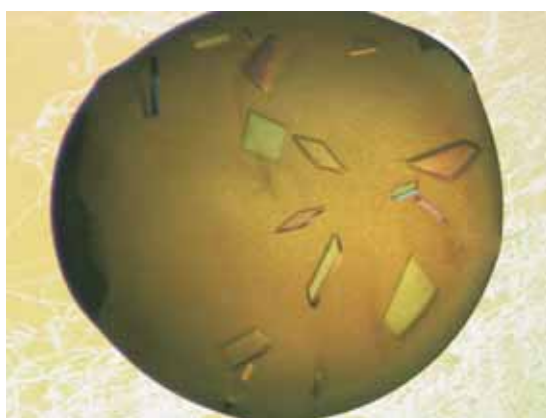
RESEARCH ACTIVITIES

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 the research projects bear the following titles: "Micro- and nano-particles in biotechnology" (L4-6171), "Steroid 11beta-hydroxylase from filamentous fungus *Cochliobolus lunatus*" (L4-4353) and "Structural studies of inositol polyphosphate kinases" (J4-6463).

Research programme of Laboratory L11 includes the following research areas:

- Investigation of approaches to biotechnological production of recombinant cytokines
- Cell biology of yeast *Saccharomyces cerevisiae*
- Biotechnology of lower eucaryotes (filamentous fungi and yeasts)

- načrtovanje in pridobivanje novih, delno spremenjenih proteinskih molekul z izboljšanimi lastnostmi za uporabo ali za lažje pridobivanje
- Proteinski laboratorij: 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 citokinov
 - Genomika in proteomika: kvasni dvo-hibridni sistem za ugotavljanje celičnih interakcij "protein-DNA" oz. "protein-protein"
 - Lokalizacija celičnih proteinov s fluorescenčno mikroskopijo
 - Preučevanje tri-dimenzionalnih struktur biološko aktivnih molekul z X-žarkovno kristalografijo in nuklearno magnetno resonanco (NMR).
- BIBLIOGRAFIJA**
- 10 izvirnih znanstvenih člankov
 - 1 pregledni znanstveni članek
 - 4 intervjuji
- Study and gene cloning of steroid bioconverting enzymes in filamentous fungi
 - Structural studies of biologically active molecules
- 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
 - Genomics and proteomics: yeast two-hybrid system for assessing cellular "protein-DNA" and "protein-protein" interactions
 - Protein cellular localisation by fluorescence microscopy
 - Three-dimensional structure determination of biologically active molecules by X-ray crystallography and nuclear magnetic resonance (NMR)



SLIKA 1:
Kristali encima iz bakterije *Mycobacterium tuberculosis*

FIGURE 1:
Crystals of an enzyme from *Mycobacterium tuberculosis*

- 2 objavljena znanstvena prispevka na konferencah (vabljeni predavanja)
- 1 objavljen strokovni prispevek na konferenci (vabljeni predavanja)
- 2 objavljena znanstvena prispevka na konferencah
- 26 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 3 objavljeni povzetki strokovnih prispevkov na konferencah
- 5 patentnih prijav
- 3 patenti
- 1 predavanje na tuji univerzi
- 1 prispevek na konferenci brez natisa
- 4 diplome
- 2 doktorata

DOSEŽKI V LETU 2005

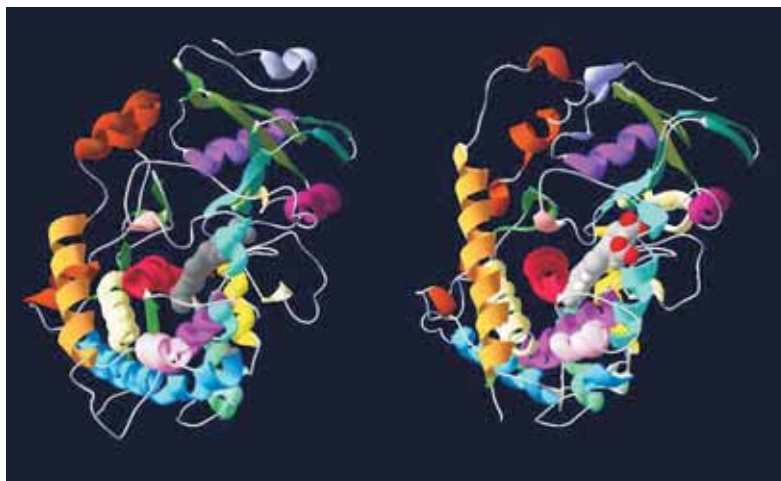
- Oblikovali smo nov pristop biosinteze rekombinantnih proteinov v bakteriji *E. coli*, ki poteka pod posebnimi pogoji in vodi do tvorbe zanimivih proteinskih agregatov z visokim deležem pravilno zvitega tarčnega proteina oziroma njegovega prekursorja. V nasprotju z običajnimi »klasičnimi« inku-

BIBLIOGRAPHY

- 10 Original Scientific Articles
- 1 Review Article
- 4 Interviews
- 2 Published Scientific Conference Contributions (Invited Lecture)
- 1 Published Professional Conference Contribution (Invited Lecture)
- 2 Published Scientific Conference Contributions
- 26 Published Scientific Conference Contribution Abstracts
- 3 Published Professional Conference Contribution Abstracts
- 5 Patent Applications
- 3 Patents
- 1 Invited Lecture at a Foreign University
- 1 Unpublished Conference Contribution
- 4 Undergraduate Theses
- 2 Doctoral Dissertations

IMPORTANT ACHIEVEMENTS IN 2005

- A new approach to recombinant protein production in *E. coli* was developed. Biosynthesis of recombinant proteins at low tempera-



SLIKA 2:

Model trodimenzionalne strukture kloniranega citokroma P450 iz nitaste glive *Cochliobolus lunatus* (D) v primerjavi s poznano strukturo človeškega citokroma P450 3A4 (L).

FIGURE 2:

Model of 3D-structure of cytochrome P450 cloned from the filamentous fungus *Cochliobolus lunatus* (R) in comparison to the known structure of human cytochrome P450 3A4 (L).

zijskimi telesi smo za ta bolj topna inkluzijska telesa, iz katerih lahko z blago ekstrakcijo pridobimo aktivno obliko tarčnega proteina, uvedli pojem »neklasična« inkluzijska telesa. Medtem ko običajen način pridobivanja heterolognih proteinov iz inkluzijskih teles *E. coli* navadno vključuje uporabo močnih denaturantov in reducentov, čemur sledi bolj ali manj uspešna faza renaturacije predhodno popolnoma denaturiranega proteina, lahko ekstrakcijo proteina iz »neklasičnih« inkluzijskih teles izvedemo v nedenaturirajočih pogojih. Raztapljanje »neklasičnih« inkluzijskih teles poteka v primernih pufrih, ob dodatku nizkih koncentracij blagih detergentov ali polarnih topil oziroma nede-tergentnih sulfobetainov, pri čemer ekstrahiramo do 45% celokupno prisotnega proteina v biološko aktivni obliki. Prisotnost pravilno zvitega proteina G-CSF v inkluzijskih telesih, nastalih pod pogoji sinteze pri nizkih temperaturah, smo potrdili z meritvami biološke aktivnosti in FT-IR spektralno analizo, s poskusi na drugih proteinih (GFP, TNF β in njegovi analogi, specialni histidinski analogi TNF α s histidinskim podaljškom, pripetim na skrajšan N-konec molekule) pa smo dokazali, da je koncept »neklasičnih« inkluzijskih teles bolj splošen in verjetno uporaben tudi za enostavno pridobivanje drugih proteinov.

- Na primeru treh različnih oblik dejavnika tumorske nekroze beta (TNF β) smo preučevali vpliv strukture in dolžine N-terminalnega dela molekule na fizikalno-kemijske lastnosti proteinov. V bakteriji *E. coli* smo pripravili MetTNF β , ki je služil kot primerjalna substanca z naravno strukturo, in dva analoga TNF β , ki imata nekoliko spremenjen N-terminalni del molekule. His7TNF β je daljša oblika proteina s heptahistidinskim podaljškom, pripetim na naravni N-konec, medtem ko ima Δ N19TNF β skrajšan N-terminalni del molekule. Podobno kot v predhodnih raziskavah strukturno sorodnega proteina TNF α , smo ugotovili, da lahko s pripenjanjem histidinskih podaljškov na hidrofobne regije

ture leads to the formation of interesting protein aggregates, containing a high amount of properly folded target protein (or its precursor). These inclusion bodies are more fragile and more soluble than "classical" ones, thus a new term "nonclassical" inclusion bodies was proposed. While protein isolation from "classical" inclusion bodies requires a series of denaturation / renaturation steps with relative low efficiency, higher solubility and fragility of "nonclassical" inclusion bodies enables extraction of biologically active target protein by mild extraction under non-denaturing conditions. "Nonclassical" inclusion bodies are solubilized in adequate buffers containing low concentration of mild detergents, polar solubilisers or non-detergent sulfobetains, and up to 45% of total target protein is extracted in biologically active form. Presence of correctly folded G-CSF inside "nonclassical" inclusion bodies was confirmed by FT-IR spectral analysis as well as with biological activity determinations. Studies on other proteins (GFP, TNF β and its analogs, analogs of TNF α with histidine tag on N-terminus) confirmed that the concept of "nonclassical" inclusion bodies is more general and thus useful for simple cost-effective downstream processes in biotechnology.

- We studied the relationship between the N-terminal protein structure and its physico-chemical properties using three different forms of tumor necrosis factor beta (TNF β). All three proteins were designed and expressed in *E. coli*. MetTNF β represented the reference substance, His7TNF β was the longer form bearing a hepta-histidine tag attached to the natural N-terminus, and Δ N19TNF β possessed a shortened N-terminal part. Similarly as in the case of the structurally related protein TNF α , we concluded that attachment of His patches to the hydrophobic regions of the protein affects its solubility and consequently distribution of the protein between the soluble and insoluble fraction of the cell.

- proteina vplivamo na topnost proteina in s tem na delež topnega proteina v citoplazmi oziroma na delež proteina v netopnih inkluzijskih telesih.
- Na primeru trimernega proteina TNF α smo preučevali tudi uporabnost različnih histidinskih podaljškov za enostavno čiščenje proteina, s poudarkom na odstranitvi afinitetnih podaljškov po učinkoviti izolaciji proteina. Za farmacevtsko uporabne proteine je namreč nujna avtentična struktura, zato mora biti encimatska odstranitev afinitetnih podaljškov čim bolj učinkovita, obenem pa mora zagotavljati pravilno procesiranje, da ne pride do heterogenosti na terminalnih delih molekule. Nepopolna odstranitev afinitetnih podaljškov znižuje končne izkoristke pri pridobivanju proteina, kar je zlasti očitno pri oligomernih proteinih. Postavili smo tudi teoretični model o vplivu oligomernosti na končni izkoristek, ki smo ga eksperimentalno potrdili s kromatografsko ločbo mešanih trimerov, nastalih ob namerem dodatku His7-dN6LK-805 k očiščenemu proteinu dN6LK-805.
 - V poročilu za leto 2004 smo že omenili, da smo iz nitaste glive *C. lunatus* uspeli izolirati gen za enega od njenih citokromov P450. Gen smo sedaj izrazili v bakteriji *E. coli* in funkcionalnost proteinskega produkta potrdili z diferencialnimi CO-spektri ter z rekonstitucijo hidroksilaznega kompleksa z zajčjo P450-reduktazo *in vitro*. Funkcijska analiza je pokazala, da gre za benzoatni-p-hidroksilazi podoben protein. Računalniški model 3D-strukture je pokazal, da se ta citokrom P450 v nekaterih površinskih strukturalnih zankah precej razlikuje od struktur poznanih citokromov P450, kar nudi lepe perspektive za iskanje specifičnih inhibitorjev. V teku so poskusi kristalizacije proteina, prečiščenega z afinitetno kromatografijo. Iz genomske knjižnice glive *C. lunatus* smo pridobili še eno delno zaporedje nekega citokroma P450 z neznano funkcijo ter obe citokromski reduktazi, CPR-1 in CPR-2.
 - The use of different histidine tags for efficient purification of the recombinant protein was studied on the case of the trimeric TNF α protein, with special focus on the removal of affinity tags after purification. For pharmaceutical proteins the authentic structure is required, enzymatic removal should therefore be very efficient and on the other hand, it should assure correct processing in order to avoid heterogeneity on the terminal parts of the molecule. Incomplete removal of affinity tags significantly reduces final yields of protein purification, which is especially obvious with oligomeric proteins. Theoretical model was set, describing the influence of the degree of oligomericity on the final yield, and was experimentally proven by the separation of mixed trimers that were formed by intentional addition of different amounts of His7-dN6LK-805 to the purified dN6LK-805.
 - As already mentioned in the annual report for 2004, one of the P50 cytochrome genes from the filamentous fungus *C. lunatus* was isolated. The gene was recently expressed in the bacterium *E. coli*, the functional activity of protein product was confirmed with differential CO-spectra and the hydroxylase complex was reconstituted with rabbit P450-reductase *in vitro*. This P450 cytochrome was characterized as benzoate-p-hydroxylase-like protein. A computer 3D-structure model has shown some interesting differences in surface structure loops of the protein with those of known P450 cytochrome structures, which can be very helpful in searching for specific inhibitors. Crystallization experiments of the protein purified with affinity chromatography are in progress. From the genome library of *C. lunatus* a partial sequence for another P450 cytochrome with unknown function was obtained, as well as genes for two cytochrome P450 reductases, CPR-1 in CPR-2. Expression experiments of both reductase genes are in progress and will be followed by reconstitution experiments with benzoate-p-hydroxylase-like protein. Studies of

Poskusi ekspresije obeh reduktaznih genov so v teku; oba proteina bomo okarakterizirali v rekonstituciji z že omenjeno benzoatno-p-hidroksilazo ter nadaljevali z ugotavljanjem inducibilnosti komponent hidroksilaznega sistema. S supresivno subtraksijsko hibridizacijo smo pridobili odzemno cDNA knjižnjico in med nukleotidnimi zaporedji 452 klonov odkrili 2 zaporedji, podobni hidroksisteroidni 17beta-dehidrogenazi, ter 12 zapisov za citokrome iz družine P450, od teh kar 7 podobnih glivnim citokromom z neznano funkcijo. Nadaljujemo z izolacijo ustreznih cDNA in funkcijskimi analizami. Omenjene poskuse spremljajo tudi poskusi utišanja genov v glivi *C. lunatus*, da bi ugotovili njihovo esencialnost, kot podlago za konstrukcijo ustreznih inhibitorjev omenjenega fitopatogenega in oportunega človeško patogenega mikroorganizma. Nadaljujemo tudi s poskusi direktnega iskanja samega gena za steroidno 11beta-hidroksilazo.

- V sklopu preučevanja molekul, ki sodelujejo pri prenosu signalov s pomočjo cikličnih nukleotidov, nas predvsem zanimajo biokemijske in strukturne značilnosti fosfodiesteraz, ki razgrajujejo ciklične nukleotide. Na tem področju sodelujemo s skupino prof. dr. Visweswariah z Indian Institute of Science iz Bangalorja v Indiji. Rekombinantne proteine iz bakterije *M. tuberculosis* smo izrazili v *E. coli* ter jih izolirali in očistili v zadostnih količinah za kristalografske in ostale biofizikalne raziskave. Očiščene proteine smo kristalizirali; določevanje in analiza kristalnih struktur je v teku.
- Študije inozitol heksakis-fosfatne kinaze smo razširili z enega encima na vse tri obstoječe izooblike. Izdelali in optimizirali smo metodo za ekspresijo rekombinantnih sesalskih proteinov v *E. coli* ter razvili metodo izolacije čistih proteinov za nadaljnje biokemijske in biofizikalne študije. Naše raziskave so bile usmerjene v podrobne študije encimskih

inducibility of different components of the hydroxylase system are in progress. With suppressive subtraction hybridization 452 nucleotide sequences were obtained, among them 2 sequences similar to hydroxysteroid 17-beta-dehydrogenase, and 12 sequences of the P450 cytochrome family, 7 out of them similar to fungal cytochromes with unknown function. We continue with isolation of adequate cDNA and functional analyses. These experiments are coupled with gene deletion experiments in the fungus *C. lunatus*, to find out whether these genes are essential, which could further aid the construction of suitable inhibitors for this phytopathogen and opportunistic human pathogenic microorganism. We continue also with alternative approaches to discover the gene for steroid 11beta-hydroxylase.

- In the last year we have expanded our studies of the inositol hexakisphosphate kinase (IP6K) from one to all three known isoforms of this enzyme. We established a protocol for the expression and purification of the mammalian enzymes in *E. coli*. The purified enzymes were used further in the biochemical and biophysical studies. We extensively studied the *in vitro* enzymatic reactions, analyzed them and compared the product formation by all three enzymes. Additionally, we purified the major product of the kinase reaction and its structure was analyzed by the nuclear magnetic resonance (NMR). This is the first structural analysis on the product of the IP6K reaction so far. This product is a pyrophosphate form of the fully phosphorylated inositol ring that is known to be involved in the phosphorylation of other proteins. Other physico-chemical features of these molecules are currently under study.
- Within this project studying the signal transduction *via* cyclic nucleotides as the second messengers, we are particularly interested in the biochemical and structural features of the phosphodiesterases, enzymes that degrade

reakcij teh encimov, predvsem v primerjalno analizo produktov (do sedaj sta znana dva možna produkta) pri vrsti raznolikih pogojev encimske reakcije *in vitro*. Izolirali smo glavni produkt vseh treh kinaz in ga analizirali z nuklearno magnetno resonanco (NMR), kar je do sedaj prva strukturna analiza tega produkta. Študije ostalih fizikalno-kemijskih lastnosti teh molekul so v teku.

- V sklopu raziskav celičnega cikla pri kvasovki *S. cerevisiae* smo pokazali, da je gen *ECM11* pomemben del zapletene mreže genov, vpletenih v sporulacijo, čeprav je po podatkih iz literature uvrščen med gene, vpletene v biosintezo celične stene. Ugotovili smo, da v kvasovki gen *ECM11* vpliva na procese mejotične replikacije, mejotične rekombinacije in na segregacijo kromosomov. Z analizo naših rezultatov smo ugotovili, da pri sevih z okvarjenim genom *ECM11* pride do napak pri mejotičnem prekrížanju, kar je vzrok za spremembe pri segregaciji kromosomov med mejozo I in za spremembe pri konverziji genov v teh sevih. Pokazali smo, da se količina proteina Ecm11, ki je med mejozo zelo verjetno vezan na protein Smt3 (sumoiliran), močno poveča med procesom sporulacije.
- Kljub velikemu številu novih ekspresijskih sistemov, kvasovka *S. cerevisiae* ostaja pomemben gostitelj za pridobivanje različnih heteroloških proteinov. Promotorske sekvence genov *GAL1*, *GAL7* in *GAL10*, ki omogočajo visoko ekspresijo teh genov, sodijo med najbolj preučene in so pomembne za načrtovanje in konstrukcijo vektorjev. Z lastno analitsko metodo za kvantitativno preiskovanje velikega števila različnih kvasnih mutant *in vivo*, smo ugotovili, da sta za ekspresijo iz promotorja *GAL1*, najpomembnejša proteina Gal1 in Gal4. Z gensko manipulacijo smo lokus gena *GAL1*, ki kodira encim galaktokinaza, zamenjali z genom za transkripcijski aktivator Gal4. Načrtovana zamenjava genov je v mutiranem sevu povzročila bistveno izboljšanje specifične produktivnosti rekombinantnih proteinov, ki

cyclic nucleotides. This project is a collaboration with a group of Prof. Dr. Visweswariah from Indian Institute of Science in Bangalore, India. We have expressed the recombinant proteins from *M. tuberculosis* in the laboratory strain of *E. coli*. The proteins were produced and purified in the quantities sufficient for the crystallographic and other bio-physical studies. The purified proteins were crystallized and the determination and analysis of the crystal structures is currently in progress.

- Ecm11 is classified as a protein involved in yeast cell wall biogenesis and organization, but we provided evidence that it is involved in meiosis as well. We found out that mutants with deleted *ECM11* exhibit complex defects in meiosis: replication, recombination and chromosome segregation are affected. Summarising our data, we concluded that the absence of the functional *ECM11* gene product affects meiotic crossing-over resulting in abnormal gene conversion and chromosome segregation in meiosis I. Additional results showed that the amount of Ecm11 protein in the cell is elevated significantly during meiosis.
- Yeast *S. cerevisiae* is an attractive host organism for production of foreign proteins, despite of large number of newly designed expression system. Well-studied *GAL1*, *GAL7* and *GAL10* promoters, enabling high expression of these genes, are important for design and construction of yeast plasmids. With own analytical procedure for quantitative screening of large number of yeast mutant *in vivo*, we have demonstrated that Gal1 and Gal4 are the most important proteins for expression of heterologous genes driven by galactose-inducible promoter. Using recombinant DNA techniques, *GAL1* gene, encoding galactokinase, was replaced by transcriptional activator *GAL4*. The described replacement of *GAL* genes significantly improved specific productivity of recombinant proteins. Therefore, newly designed *GAL* recombinant

se izražajo pod kontrolo promotorja GAL1. Opisana zamenjava genov GAL v genomu, omogoča pripravo visoko-produkcijskih rekombinantnih sevov *S. cerevisiae*, ki so primerni za ekspresijo industrijsko (farmaceutsko) zanimivih proteinov.

- V letu 2005 je bila naša programska skupina (P1-0104 "Funkcijska genomika in biotehnologija za zdravje") uvrščena med 19 najboljših raziskovalnih programskih skupin v Sloveniji oz. s strani Agencije za raziskovalno dejavnost RS (ARRS) proglašena za najboljšo programsko skupino v letu 2004 na področju naravoslovja.

strain should prove useful for maximal expression of industrially (pharmaceutical) interesting proteins.

- In 2005 the research program P1-0104 "Functional Genomics and Biotechnology for Health" was considered by the Slovenian Agency for Research as being among the top 19 research programs in Slovenia, and the program research group was nominated the best in the field of life sciences in 2004.
- Program research group P1-0104 is also the leading group of the inter-institutional centre of excellence "Biotechnology with Phar-



SLIKA 3:
Fermentacijski laboratorij na Kemijskem inštitutu - z bioreaktorji za pridobivanje rekombinantnih proteinov v mikroorganizmih

FIGURE 3:
Fermentation Laboratory of the National Institute of Chemistry equipped with bioreactors for microbial production of recombinant proteins

- Programska skupina P1-0104 je tudi nosilna skupina medinstitucionalnega centra odličnosti "Biotehnologija s farmacijo". Ustanovitev tega centra je bila usklajena z uvrstitvijo področja "biotehnologija s farmacijo" med prioritete Evropskega sklada za regionalni razvoj in s tem povezanega razpisa Vlade RS za sredstva evropske strukturne politike. Združili smo slovenski znanstveno-raziskovalni potencial, ki izkazuje najvišjo raven odličnosti na področju nove biotehnologije, ima dolgoletno tradicijo povezovanja in tudi tekoča sodelovanja z našo farmacevtsko industrijo in vstopa na v EU prioriteto področje funkcijske genomike in biotehnologije za zdravje. Poglavitni strateški cilj ustanovitve centra odličnosti z 19 partnerji, ki pokrivajo celotno paleto znanj na širšem področju farmacije in biotehnologije, je premagovanje medinstitutskih ovir in s tem kontinuirno, dolgoročno povezovanje ter nadgradnja in zagotavljanje infrastrukture, tehnologij in vrhunskih znanj, kar naj bi ustvarilo inovacijsko okolje, ki bo primerljivo z ostalimi državami EU. V okviru centra odličnosti L11 vodi enega od dveh njegovih projektov, in sicer projekt RR2 "Načrtovanje, karakterizacija in pridobivanje biofarmacevtikov".
- V maju 2005 je bil na Medicinski fakulteti Univerze v Ljubljani slovesno odprt "Center za funkcijsko genomiko in bio-čipe" (CFGBC). Ta infrastrukturni center je nacionalnega pomena, deluje po načelu odprtega dostopa in je v lasti slovenskega konzorcija za bio-čipe, katerega član je tudi Kemijski inštitut. Vodja L11 je predsednik upravnega odbora CFGBC.

SODELOVANJE Z INDUSTRIJO

Laboratorij združuje raziskovalce Kemijskega inštituta in podjetja Lek d.d., Biofarmaceutika, Rekombinantna biotehnologija, Ljubljana, tako da gre za mešano skupino, ki že vrsto let deluje na skupnih raziskovalnih projektih.

macy" which was established, as one of the nine priorities, following the call of the Government of Republic Slovenia for funding by the European Funds for Regional Development. The vast majority of Slovenian research potential was gathered together expressing the highest level of excellence in the field of new biotechnology associated with EU priorities such as functional genomics and biotechnology for health, and also expressing traditional collaboration with the pharmaceutical industry. The main strategic objective of the 19 partners of the Centre is continuous long-term research collaboration and setting-up joint infrastructural facilities following recent progress in science and technology, and thus setting up innovative post-genomic environment concent with those in other EC countries. Laboratory L11 is coordinating one of the two research projects of the Centre, namely project RR2 – Design, characterization and production of biopharmaceuticals.

- In May 2005 the Slovenian Consortium for Microarray Technology inaugurated, at the Faculty of Medicine, University of Ljubljana, Slovenia, the "Centre for Functional Genomics and Bio-chips" (CFGBC). The Centre operates as national infrastructural facility and is coordinated by steering committee of representatives from the 12 members of the Consortium. Head of the L11 as representative of the NIC was elected president of the CFGBC Steering Committee.

COLLABORATION WITH INDUSTRY

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

MEDNARODNO SODELOVANJE IN POVEZAVE

- FW6-2004-NMP-NI-4; IP 026723-2 NANO-BIOPHARMACEUTICS: Integrated FW6 Project "Nanotechnology-based Targeted Drug Delivery" (V. Gaberc Porekar, V. Menart-partnerstvo pri projektu; 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 - član Znanstvenega sveta ICGEB (CSA - Council of Scientific Advisers; prvi mandat 2004 - 2007)
- European Science Foundation: R. Komel - član upravnega odbora znanstvenega programa ESF "Integrated Approaches for Functional Genomics" (2004 - 2006)
- 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, ZDA: sodelovanje z dr. Rashna Bhandari iz laboratorija prof. Solomona Snyderja na projektu "Strukturne raziskave inozitol polifosfatnih kinaz" (M. Podobnik)

POMEMBNI 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

INTERNATIONAL ACTIVITIES AND COLLABORATION

- FW6-2004-NMP-NI-4; IP 026723-2 NANO-BIOPHARMACEUTICS: 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)
- European Science Foundation: R. Komel - ESF Programme "Integrated Approaches for Functional Genomics"; Steering Committee Member (2004 - 2006)
- EC Network of Excellence NANOFUN-POLY (V. Menart, V. Gaberc Porekar – membership in 2004 - 2007)
- Indian Institute of Science, Bangalore, India: collaboration with Prof. Sandhya Visweswariah; project "Structural Studies of cAMP-phosphodiesterase from *M.tuberculosis*" (M. Podobnik)
- Johns Hopkins University Medical School, Baltimore, USA: collaboration with Dr. Rashna Bhandari from the laboratory of Prof. Solomon Snyder on the "Structural studies of inositol poly-phosphate kinases" project (M. Podobnik)

MAJOR EQUIPMENT

- Laboratory for gene technology
- Laboratory for isolation, purification and characterisation of (recombinant) proteins
- Laboratory for cell cultures
- Laboratory for microbiology
- Laboratory with bio-reactors

Vsi omenjeni laboratoriji so ustrezno opremljeni za izvajanje navedenih projektov, kot pomembnejše pa posebej navajamo naslednjo opremo:

- pretočni citometer z možnostjo sortiranja celic (Beckman Coulter, konzorcij)
- fluorescenčni mikroskop (Zeiss) s sistemom za slikanje
- stereo mikroskop (Nikon)
- fluorimeter (PTI)
- 2 UV/VIS spektrofotometra (Agilent, Hewlett-Packard)
- CD-spektrometer "Chirascan CD Spectrometer" (Applied Photophysics, konzorcij)
- Dynamic Light Scattering Detector (DynaPro)
- sistem za denzitometrijo ProExpress Imaging System (Perkin Elmer)
- izotermalni titracijski kalorimeter (MicroCal, konzorcij)
- 4 preparativni sistemi za kromatografsko ločevanje proteinov (Amersham Biosciences, Knauer)
- 1 analitski HPLC sistem (Waters)
- 2 računalniško vodena laboratorijska bio-reaktorja (Applikon)
- 2 sistema za pripravo Milli-Q vode (Millipore)
- sistem za dokumentacijo gelov (Chemi Doc, BIO-RAD)
- hladilne kapacitete +4°C, -20°C in -70°C
- 4 stresalniki
- sklop aparatov za pomnoževanje in sekvencno analizo DNA

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, consortium)
- Fluorescence microscope with CD camera (Zeiss)
- Stereo microscope (Nikon)
- Fluorimeter (PTI)
- 2 UV/VIS spectrophotometers (Agilent, Hewlett-Packard)
- Chirascan CD Spectrometer (Applied Photophysics, 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



VODJA / HEAD

Prof. dr. Roman Jerala

RAZISKOVALCI / RESEARCHERS

Dr. Mojca Benčina
Dr. Jožefa Friedrich
Dr. Helena Gradišar
Prof. dr. Nina Gunde-Cimerman
Dr. Katarina Jernejc
Prof. dr. Matic Legiša
Dr. Andreja Majerle
Dr. Mateja Manček Keber
Dr. Primož Pristovšek

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Tanja Bagar
Iva Hafner Bratkovič
Lorena Butinar
Boštjan Japelj
Tina Mlakar
Martina Mohorčič
Gabrijela Panter
Nina Pirher
Nuša Resman
Mireille Treeby
Aleksandra Usenik
Jožica Vašl
Mateja Zorko

TEHNIČNO OSEBJE / TECHNICAL STAFF

Robert Bremšak
Darija Oven
Irena Škraba



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, farmacevtsko). 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 molekulskih 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 disease 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 its own Microbial Culture Col-

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

BIBLIOGRAFIJA

- 18 izvirnih znanstvenih člankov
- 1 kratki znanstveni prispevek
- 1 samostojni znanstveni sestavek v monografiji
- 3 objavljeni znanstveni prispevki na konferencah
- 23 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 patentna prijava
- 1 patent
- 5 predavanj na tujih univerzah
- 1 prispevek na konferenci brez natisa
- 8 diplom
- 1 doktorat

GLAVNI DOSEŽKI V LETU 2005

V letu 2005 smo v sodelovanju z drugimi laboratoriji na Kemijskem inštitutu in zunanjimi uporabniki pridobili pretočni citometer s sorterjem in CD spektrometer, dve pomembni aparaturi za raziskave v molekularni in strukturni biologiji.

V zvezi z raziskavami receptorjev LPS oz. inhibicijo signalizacije Toll-u podobnih receptorjev (TLR) smo v lanskem letu napravili pomemben korak naprej, saj smo s pomočjo fluorescenčnih prob pokazali na pomen hidrofobnih interakcij pri prepoznavanju in na tej osnovi testirali vezavo vrste spojnin, za katere je bilo prej že ugotovljeno, da inhibirajo celično signalizacijo preko NF- κ B. Vlogo hidrofobnih interakcij v vezavnem žepu smo potrdili tudi z usmerjenimi mutantami MD-2, ki je vezan na izvenselično domeno TLR4. Vezavo enakih spojnin kot na MD-2 smo analizirali tudi na homologa Der p2 in GM2-AP in ugotovili, da je GM2-AP najbrž bolj primeren strukturni model za MD-2.

Poleg inhibicije receptorja lahko nevtralizacijo delovanja endotoksina dosežemo tudi s spojinami, ki se direktno vežejo na LPS in

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

BIBLIOGRAPHY

- 18 Original Scientific Articles
- 1 Review Article
- 1 Independent Scientific Component Part in a Monograph
- 3 Published Scientific Conference Contributions
- 23 Published Scientific Conference Contribution Abstracts
- 1 Patent Application
- 1 Patent
- 5 Invited Lectures at Foreign Universities
- 1 Unpublished Conference Contribution
- 8 Undergraduate Theses
- 1 Doctoral Dissertation

IMPORTANT ACHIEVEMENTS IN 2005

In 2005 a flow cytometer with cell sorting ability and a CD spectrometer were purchased with the help of other Laboratories of the National Institute of Chemistry as well as other users. The new equipment is very important for research in molecular and structural biology.

In the research field on LPS receptors or inhibition of signalization by Toll-like receptors (TLR) an important step forward was achieved. With the help of fluorescent probes we succeeded to prove the importance of hydrophobic interactions in recognition of LPS and on this basis we tested binding of a number of compounds, previously known to inhibit cell signalization via NF- κ B. The role of hydrophobic interactions in the binding pocket was confirmed also with point mutations of MD2, which is associated to the extracellular domain of TLR4. The binding of the same compounds as on MD2 was also analyzed on the homologues Der p2 and GM2-AP and found that GM2-AP is probably a more suitable structural model for MD2.

In addition to receptor inhibition it is possible to neutralize the endotoxin activity also by com-

preprečijo njegovo vezavo na receptorje. Določili smo 3D strukturo več kot štirim peptidom, bodisi v okolju membranskih mimetikov ali LPS. Analizirali smo tretjo generacijo peptidov, ki so imeli bistveno izboljšano antimikrobno delovanje in smo jih zasnovali na osnovi 3D strukture peptidov v kompleksu z LPS in v micelah kot membranskih mimetikih. Ugotavljali smo vpliv acilacije peptida na spremembo aktivnosti in interakcijo z membranami ter njegovo 3D strukturo v zwitterionskih micelah. Na osnovi rezultatov antimikrobnega delovanja in nevtralizacije endotoksina skupaj s partnerji EU projekta pripravljamo prijavo mednarodnega patenta in nato objavo rezultatov.

Na raziskavah prionskih proteinov smo v lanskem letu napredovali tudi na področju vezave spojin, ki se vežejo na amiloide, kjer smo ugotovili tudi delovanje in način vezave spojin naravnega izvora, kot je kurkumin, kar lahko vodi k novim zdravilom in/ali diagnostiki. Na tem področju smo intenzivno vključeni v mednarodno sodelovanje in smo začeli z izvajanjem EU projekta TSEUR.

Na področju načrtovanja primarnega metabolizma smo v preteklem letu zaključili s koordinatorskim evropskega projekta ANTICO, ki ga je tri leta sofinancirala Evropska komisija pod okriljem 5. Okvirnega projekta. Namen projekta je bilo dokazati, da lahko s prenosom dveh ključnih genov, izoliranih iz glive *Aspergillus niger*, ki kodirajo encime primarnega metabolizma, v druge komercialne mikroorganizme dvignemo produktivnost slednjih. Praktično pri vseh recipientskih mikroorganizmih, tako filamentoznih glivah, kvasovkah in bakterijah, smo uspeli, vsaj v enem primeru, dokazati pozitiven učinek vnešenih genov na povečano produkcijo. Še najboljše rezultate pa smo dobili z vnosom skrajšanega gena za kratek fragment 6-fosfofrukto-1-kinaze (PFK1). Pred kratkim smo namreč ugotovili, da pri glivi *Aspergillus niger* pride do posttranslacijske modifikacije nativnega encima, pri tem pa nastane krajši fragment encima s spremenjeno kinetiko. Bistvena prednost novo nastalega

pounds that directly bind to LPS and prevent its binding to receptors. We determined 3D structure of more than four peptides either in the presence of membrane mimetics or LPS. We analyzed the third generation of peptides showing essentially improved antimicrobial activity and were prepared on the basis of the 3D structure of peptides in the complex with LPS and in micelles as membrane mimetics. We also investigated the effect of acylation of the peptide on the activity and interaction with membranes as well as its 3D structure in zwitterion micelles. Based on the results of antimicrobial activity and of endotoxin neutralization we are preparing, together with our partners in the EU project, an international patent application and subsequent publication of the results.

In the research of prion proteins a progress was made in the field of binding compounds that bind to amyloids. We elucidated the action and the mode of binding of natural compounds such as curcumin, which could lead to discovery of new drugs and/or diagnostic tools. In this research field we are intensively involved in the international cooperation and we just started the work on EU project TSEUR.

In the field of designing primary metabolism in 2005 we brought to the end a coordination of the EU project ANTICO which was financed by the EC in the 5 FW program for three years. The aim of the project was to prove that it was possible to improve the productivity of commercial microorganisms by transferring two key genes from the fungus *Aspergillus niger* coding for enzymes of primary metabolism. Almost in all recipient microorganisms, filamentous fungi, yeasts and bacteria, we succeeded to prove, at least in one case, a positive effect of the introduced genes on increased production. The best results were obtained by the introduction of a shortened gene for a short fragment of 6-phosphofructo-1-kinase (PFK1). Recently, we found that with the fungus *A. niger* a posttranslational modification of the native enzyme occurred, which resulted in a shortened

encima je sposobnost aktivacije ob prisotnosti specifičnih celičnih aktivatorjev, medtem ko je rezistenten na inhibicijo s citratom. O posttranslacijski modifikaciji 6-fosfofrukto-1-kinaze, tega ključnega regulatornega encima glikolize, smo objavili članek v ugledni znanstveni reviji. Pripravili smo skrajšan gen, ki je po transformaciji v glivine celice neposredno sintetiziral krajši fragment. Transformanti gliv *A. niger* in *A. terreus*, ki so nosili integriran gen za krajši fragment, so bili sposobni hitrejše sinteze končnih produktov. Pozitivni efekt vnosa gena za krajši fragment se je pokazal tudi pri produkciji heterolognih proteinov pri kvasovki *Pichia pastoris*. Zaradi izredne uporabne vrednosti rezultatov pridobljenih s projektom ANTICO, se je konzorcij raziskovalcev iz petih evropskih inštitucij odločil, da bo izsledke patentno zaščitil. Istočasno se pripravljamo tudi na navezavo stikov z uporabniki iz različnih, primarno evropskih biotehnoških družb, s katerimi nameravamo začeti pogovore o licenciranju.

Pri glivi *Aspergillus niger* smo ločili dva izoenzima NADP-odvisne izocitrat dehidrogenaze. Encima imata različne kinetične lastnosti in različno lokacijo v celici. Med izoenzimoma so izrazite razlike v velikosti in stopnji aktivacije ter stopnji inhibicije ob prisotnosti različnih metabolitov.



SLIKA 1:

Gram-negativna bakterija *Escherichia coli*, kateri je bil na desni sliki dodan antimikrobni peptid, ki povzroči opazne poškodbe bakterijske celične stene. Sliko sta z elektronskim mikroskopom na Kemijskem inštitutu posneli Lorena Butinar in Mateja Zorko.

fragment of the enzyme with a changed kinetics. The essential advantage of the new form of enzyme was the ability of activation in the presence of specific cell activators, while it was resistant to inhibition by citrate. About the posttranslational modification of PFK1, the key regulatory enzyme in glycolysis, we reported in a publication in a recognized international journal. We prepared a shortened gene that directly synthesized the shorter fragment after transformation into fungal cells. The transformants of *A. niger* and *A. terreus* having the integrated gene for the shorter fragment were able to synthesize the final products in shorter time. The positive effect of the introduction of the gene for the shorter fragment was evident also in the production of heterologous proteins in the yeast *Pichia pastoris*. Due to the outstanding applicability of the results obtained in the ANTICO project the consortium decided to patent the findings. At the same time we have contacts with the potential users, such as European biotechnological companies, to discuss about licensing.

With the fungus *A. niger* two iso-enzymes of NADP-dependent iso-citrate dehydrogenase were separated. The iso-enzymes have different kinetic characteristics and different location within the cell. Between them there are pronounced distinctions in their sizes and in their

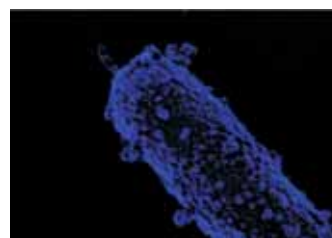


FIGURE 1:

Electron micrograph of Gram-negative bacteria *Escherichia coli*. Antimicrobial peptide has been added to the bacteria on the right panel. Large defects in the cell membrane is visible. SEM pictures were made on the instrument at the National Institute of Chemistry by Lorena Butinar and Mateja Zorko.

Pripravili smo rekombinantni senzor za spremljanje kalcija, pH in proteazne aktivnosti, ki omogočajo *in vivo* spremljanje koncentracije kalcija, vrednosti pH in aktivnost citosolnih proteaz gliv. Osnovni gradniki senzorjev so zeleni fluorescirajoči proteini. 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 senzora v glivah. Z rekombinantnim senzorjem 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. V našem laboratoriju smo pridobili keratinazo s fermentacijo s submeznim gojenjem glive v bioreaktorju in jo testirali pri naših sodelavcih v Angliji. Rezultati so pokazali, da je z encimom možno izboljšati propustnost modelne keratinske membrane. V letu 2005 smo preizkusili okrog 100 sevov gliv na izbranem modelnem substratu za Bayer-Villigerjevo reakcijo, s katerim je možno pridobiti po dve stereo in dve optični izomeri. Številne glive so bile sposobne transformirati substrat, vendar so bili produkti različni. Glede na profil in optično čistost dobljenih produktov smo glive lahko razvrstili v štiri skupine.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

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

MEDNARODNO SODELOVANJE

mednarodni projekti:

- Dva evropska projekta v okviru 5. okvirnega programa: ANTICO in ANEPID
- Dva evropska projekta v okviru 6. okvirnega programa: Eurofungbase in TSEUR

activation- and inhibition in presence of different metabolites.

A recombinant sensor for calcium, pH and proteolytic activity detection was prepared which enable *in vivo* detection of calcium concentration, pH value and activity of cytosolic proteases in fungi. Essential building blocks of the sensors are green fluorescent proteins. The calcium sensor was analyzed, in cooperation with partners from the University of Edinburgh with the FLIM-FRET (Förster resonance energy transfer in fluorescence lifetime imaging microscopy) method, confirming the possibility of application of the sensor in fungi. With the recombinant sensor for the pH we determined the intracellular pH value in fungi and we confirmed that the intracellular control was connected with the control of the intracellular calcium concentration, since in fungi with damaged calcium pumps an increase of intracellular pH occurred. In our Laboratory, a fungal keratinase was produced in a bioreactor by submerged fermentation and our British partners tested the enzyme. Results showed that by using the enzyme it was possible to increase permeability of a keratinous membrane. In 2005 we tested around 100 fungal strains on a selected model substrate, for Baeyer-Villiger oxidation, which enables the production of two stereo- and two optical isomers. Several fungi were able to transform the substrate. However, the obtained products were different. According to the profile and optical purity of the products the fungi could be classified into four different groups.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

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

INTERNATIONAL COLLABORATION

international projects:

- Two projects within the 5th Framework Programme: ANTICO in ANEPID

- Bilateralno sodelovanje s Hrvaško, Veliko Britanijo (v okviru programa Partnership in Science (4x)), Portugalsko, Italijo, Madžarsko, Indijo in Francijo (PROTEUS)
- 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:

- Technische Universität München, Nemčija
- University of Sussex, Velika Britanija
- 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
- CD spektrometer Chirascan, Applied Photo-physics
- UV/VIS spektrometer, Perkin Elmer Lambda 25
- Fluorescenčni luminometer, Perkin Elmer LS-55
- Luminometer/fluorimeter za mikrotitrsko 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)

- Two projects within the 6th Framework Programme: Eurofungbase and TSEUR

- Bilateral projects with Croatia, United Kingdom (within Partnership in Science (4x)), Italy, Hungary, Portugal, India and France (PROTEUS)

- 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

nonformal collaboration with other research institutions:

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

MAJOR EQUIPMENT

- The EPICS® ALTRA™ Flow Cytometer, Beckman Coulter
- CD spectrometer Chirascan, Applied Photo-physics
- 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

- 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
- Diplomski dela v letu 2005: 8
- Doktorska dela v letu 2005: 1
- Gostovanje podiplomskega študenta Gorana Mikluševića iz Hrvaške in podiplomske študentke Kirsten Altenbach iz Velike Britanije

M. Manček Keber je za svojo doktorsko disertacijo z naslovom: LPS-vezavni proteini: analiza lastnosti in interakcij z endotoksinom (mentor: R. Jerala), prejela kar dve nagradi:

- Krkino nagrado za doktorska dela (35. Krkine nagrade 2005, Novo mesto, 28. 10. 2005) in
- Nagrado Kemijskega inštituta za izjemno doktorsko delo (8. 12. 2005)

DOSEŽEK ODMEVEN V MEDIJIH

Članek raziskovalcev Kemijskega inštituta (*Kombinacija antimikrobne aktivnosti in nevtralizacije endotoksina z novimi oleoilamini*, z avtorji Mateja Zorko, Andreja Majerle, David Šarlah, Mateja Manček Keber, Barbara Mohar in Roman Jerala), ki so ga objavili v reviji *Antimicrobial Agents and Chemotherapy* so izbrali za predstavitev v julijski številki »ASM News«, ki je glasilo največjega svetovnega profesionalnega združenja - Ameriškega združenja mikrobiologov, ki združuje preko 42,000 mikrobiologov s celega sveta. Tukaj predstavljamo prevod teksta, ki ga je za ASM News napisal David Holzman.

»Sepsa, ki je bil neposreden vzrok smrti pokojnega papeža Janeza Pavla II., je vodilni vzrok smrti v oddelkih za intenzivno nego po vsem svetu, ker zaenkrat ni na razpolago učinkovite specifične terapije«, pravi Klaus Brandenburg iz Leibnitzovega centra za

- 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
- 8 BSc projects performed at the department have been defended in 2005
- 1 PhD thesis
- Research visits of PhD students Goran Miklušević from Croatia and Kirsten Altenbach from United Kingdom

M. Manček Keber received for her PhD thesis: LPS binding proteins: analysis of their properties and interactions with endotoxin (mentor: R. Jerala) two awards:

- Krka Prize for PhD thesis, awarded by the Krka pharmaceutical company (Krka d.d., Novo mesto, Slovenia), October 2005
- The National Institute of Chemistry Award for Exceptional Doctoral Work, presented in December 2005

ACHIEVEMENT NOTED IN THE MEDIA

Paper by the researchers of L12 and L08 (*Combination of antimicrobial and endotoxin-neutralizing activities of novel oleoilamines*) by Mateja Zorko, Andreja Majerle, David Šarlah, Mateja Manček Keber, Barbara Mohar and Roman Jerala), recently published in *Antimicrobial Agents and Chemotherapy* was selected for presentation in the July issue »ASM News«, which is the magazine of the largest professional society – American Society for Microbiology, with more 42,000 mikrobiologists from the whole world. The text below has been written for ASM News by David Holzman.

Sepsis, which was the immediate cause of the death of Pope John Paul II, is the leading cause of mortality in intensive care units, "because almost no specific therapy is available," says

medicino in bioznanosti Raziskovalnega centra Borstel v Nemčiji. Papeževo sepso, kot večino vseh primerov sepse, je povzročil endotoksin iz gram-negativnih bakterij. Imunski odziv in uporaba antibiotikov lahko iz propadajočih bakterij sprostita endotoksin. Zdravilo, ki bi lahko po eni strani uničilo gram-negativne patogene in istočasno nevtraliziralo endotoksin, je neke vrste sveti gral na področju raziskav sepse. Sedaj Roman Jerala in sodelavci s Kemijskega inštituta, Ljubljana, Slovenija poročajo o sintezi novih spojin, ki združujejo ti dve lastnosti.

»To delo prispeva k znanju o zaščitnem delovanju tovrstnih spojin, ki bi lahko bile

Klaus Brandenburg of the Leibniz-Center for Medicine and Biosciences, Research Center Borstel, Borstel, Germany. The Pope's sepsis, like most, was induced by endotoxin from gram-negative bacteria. Immune reaction and antibiotics can both cause dying bacteria to release endotoxin. A drug that could both kill gram-negative pathogens and neutralize endotoxin has been a holy grail. Now Roman Jerala and colleagues of the National Institute of Chemistry, Ljubljana, Slovenia, report the synthesis of novel oleoylamines that combine the two properties. This work "adds to the growing body of literature on the protective effects of such compounds that may be of prophylactic value in



SLIKA 2:

Fluorescenčni pretočni celični sorter omogoča ločevanje celic na osnovi njihovih lastnosti in tudi istočasne meritve večjega števila citokinov v raztopini na osnovi principa multipleksinga. Ta naprava omogoča izolacijo homogenih celičnih frakcij in analizo izražanja posameznih celičnih markerjev. Inštrument je bil kupljen s sodelovanjem L11, L12 in konzorcija slovenskih raziskovalnih organizacij

FIGURE 2:

Fluorescence cell sorter allows the separation of cells based on their specific properties as well as quantification of several components in the solution based on the multiplexing. The instrument allows the separation of homogeneous cell fractions and analysis of the level of expression of specific cellular markers. The instrument was purchased by L11, L12 and the consortium of Slovenian research organizations.

uporabljene tudi preventivno za terapijo gram-negativne sepse«, pravi Sunil David iz Univerze v Kansasu v ZDA.

»Za naravni antibiotični lipopeptid polimiksin B je že dolgo znano, da nevtralizira bakterijski endotoksin, vendar njegova toksičnost preprečuje uporabo kot sistemski antibiotik«, pravi Jerala. »Za lipopoliamine vemo, da nevtralizirajo endotoksin, ne da bi bili toksični za sesalske celice, vendar doslej znane spojine niso imele antimikrobnega delovanja«. Njegova skupina raziskuje sintetične lipopeptide, med katerimi poskušajo pripraviti takšne, ki bi posnemali polimiksin B, ob tem pa bi se izognili njegovi toksičnosti za gostiteljske celice.

»Pri naših raziskavah smo ob izvajanju kontrol opazili, da ima ena od izhodnih sestavin - oleilamin, ne pa tudi sorodne spojine, antimikrobno delovanje, kar nas je navedlo, da raziščemo strukturne zahteve za to aktivnost«, pravi Jerala. »Lipid A, neobhoden del strukture endotoksina, je zelo ohranjen med bakterijami. Z analizo njegove strukture smo ugotovili, da bi morala imeti spojina, ki bi nevtralizirala endotoksin, hidrofobno površino ter par kationskih mest na ustrezni razdalji, tako da bi se vezali na dve fosfatni skupini lipida A«.

Z upoštevanjem teh zahtev so raziskovalci sintetizirali skupino spojin in testirali njihovo delovanje na bakterije. Pokazalo se je, da je dejansko možno kombinirati tako antimikrobno aktivnost kot tudi nevtralizacijo endotoksina, dodatno pa spojine za razliko od polimiksina B presenetljivo dobro delujejo tudi proti gram-pozitivnim bakterijam.

»Predvidevamo, da bodo bakterije težko razvile odpornost proti oleoilaminom«, pravi Jerala.

»Verjetno bodo te spojine imele podobno delovanje kot naravni kationski antimikrobni peptidi, proti katerim je odpornost dokaj redka, saj je bistvena sprememba lastnosti membrane za bakterije neugodna. Bakterije, ki so odporne proti kationskim peptidom, imajo običajno nizko virulenco in jih organizem tudi lažje inaktivira s fagocitozo«.

the therapy of gram-negative sepsis,” says Sunil A. David, of the University of Kansas, Lawrence. A lipopeptide compound called polymyxin B “has long been known to neutralize bacterial endotoxin, but its toxicity prevents its use as a systemic drug,” says Jerala. Lipopolyamines had been known to neutralize endotoxin (AKA lipopolysaccharide [LPS] without toxicity to eukaryotic cells, says Jerala, but they lacked antibiotic activity. His group had been experimenting with synthetic lipopeptides, trying to find one that one mimic polymyxin B’s LPS-neutralizing without killing eukaryotic cells. “We noticed that oleylamine but not other saturated alkylamines had antimicrobial activity, which prompted us to investigate the structural requirements for the activity,” says Jerala. Part of the structure of the “lipid A” section of LPS is highly conserved across the bacteria. The details of this structure suggested that an LPS neutralizing agent should have a water-repelling surface, and a pair of “cationic interaction sites” that would be spaced such that they could interact with the two phosphate groups of lipid A. The researchers then synthesized novel oleylamines incorporating these properties, and then tested them against bacteria. The results “showed that it is indeed possible to combine both antimicrobial activity and neutralization of LPS and that surprisingly, the compounds showed also comparable activity against gram-positive bacteria. Bacteria would probably have trouble developing resistance to oleylamine antibiotics, says Jerala. “I believe that oleylamines probably would behave like cationic antimicrobial peptides, where resistance is quite rare since it is expensive for the bacteria to modify the properties of their membrane,” he says. “Bacteria resistance to cationic antimicrobial peptides usually have attenuated virulence and are more efficiently inactivated by phagocytes.”

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
Matevž Vospernik (do / until 30. 04. 2005)
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 večcevni membranskih kontaktorjev
- interpretaciji eksperimentalnih meritev na podlagi matematičnega modeliranja in optimizacije parametrov
- razvoju Pd-Cu bimetalnih katalizatorjev, uporabljenih v integriranem procesu za denitrifikacijo podtalnice
- kinetičnim in mehanističnim študijam

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 catalysts for

- 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 strukturni in elektrokemični karakterizaciji novih anodnih katalizatorjev, odpornih na CO, za uporabo v PEM gorivnih celicah
 - sintezi ter strukturni elektrokemični karakterizaciji nanokompozitnih protonsko prevodnih polimernih membran za PEM gorivne celice.
- 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

- 8 izvirnih znanstvenih člankov
- 1 strokovni članek
- 1 samostojni znanstveni sestavek v monografiji
- 2 objavljena znanstvena prispevka na konferencah
- 10 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 patent
- 2 končni poročili o rezultatih raziskav
- 1 elaborat, predštudija, študija
- 1 magisterij
- 1 doktorat
- 2 uredništvu revij

DOSEŽKI V LETU 2005

- Na primeru modelne reakcije (oksidacije mravljične kisline na Pt katalizatorju) smo določili lokacijo reakcijske cone v trifaznem membranskem katalitskem reaktorju na podlagi primerjave masnih tokov ogljikovega dioksida v reakcijskih in nereakcijskih pogojih
- Razvili smo matematični model za napoved koncentracijskih profilov reaktantov in debelino reakcijske cone v katalitskem membranskem reaktorju
- Modificirali smo procesno shemo integralnega procesa za odstranjevanje presežnih

BIBLIOGRAPHY

- 8 Original Scientific Articles
- 1 Professional Article
- 1 Independent Scientific Component Part in a Monograph
- 2 Published Scientific Conference Contributions
- 10 Published Scientific Conference Contribution Abstracts
- 1 Patent
- 2 Final Research Reports
- 1 Treatise, Preliminary Study, Study
- 1 Master's Thesis
- 1 Doctoral Dissertation
- 2 Journal Editorships

RESULTS IN 2005

- Location of the reaction zone in the three-phase catalytic membrane reactor was determined on the basis of carbon dioxide fluxes measured under reaction and non-reaction conditions, when catalytic oxidation of formic acid was employed as a model reaction
- 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

- množin nitratnega iona iz pitne vode, s čimer je drastično zmanjšana produkcija amonijevega iona kot stranskega produkta reakcije
- Določili smo kinetiko reakcije vodnega plina (water gas shift reaction, WGSR) na nanostrukturiranem $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-y}$ katalizatorju v stacionarnih pogojih in dokazali, da je proces limitiran z reakcijo oksidacije CO na medfazni meji katalizatorja in na reoksidaciji te medfazne meje s kisikom iz vode
 - V sodelovanju z L07 smo določali elektrokemijske in mehanske lastnosti ter obstojnost nove protonsko prevodne polimerne membrane za visokotemperaturne PEM gorivne celice, ki smo jo razvili in patentirali za Renault, Francija
 - V sodelovanju z L02 smo določali elektrokemijske in mehanske lastnosti ter obstojnost nove protonsko prevodne polimerne membrane za PEM gorivne celice, ki smo jo razvili v projektu APOLLON (5. OP EU)
- 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, which drastically reduces the production of ammonium ions as a by-product
 - Kinetic model of water gas shift reaction (WGSR) over a nanostructured $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-y}$ catalyst based on the redox mechanism was developed; the reaction rate limiting step was demonstrated to be the CO oxidation at the nanostructured catalyst interface and the reoxidation of this interface with oxygen from water
 - Determination of electrochemical and mechanical properties and durability of the new proton conducting polymer membrane for high temperature PEM fuel cell, which was developed and patented in collaboration with L07 in the framework of research project with Renault, Paris, France



SLIKA:

Avtomatizirani sistem za karakterizacijo heterogenih katalizatorjev (Micromeritics, model Autochem II 2920), povezan z masnim spektrometrom (Pfeiffer Vacuum, model ThermoStar) kot sekundarnim detektorjem.

FIGURE:

Automated system for heterogeneous catalysts characterization (Micromeritics, model Autochem II 2920), connected to a mass spectrometer (Pfeiffer Vacuum, model ThermoStar) employed as a secondary detector.

- V sodelovanju z L10 smo določali aktivnost in obstojnost novih anodnih katalizatorjev za PEM gorivne celice s povečano odpornostjo proti zastrupljanju s CO, ki smo jih razvili v projektu APOLLON (5. OP EU)

SODELOVANJE Z INDUSTRIJSKIMI PARTNERJI

- Renault, Pariz, Francija; Sinteza protonsko prevodnih membran za visokotemperaturne PEM gorivne celice (do 30. 07. 2005), partnerstvo, projekt po pogodbi (2001 - 2004)

MEDNARODNO SODELOVANJE

- »Waste water treatment by catalytic oxidation contactor« (WATERCATOX), RTD projekt v 5. okvirnem programu EU
- »Advanced PEM Fuel Cells« (APOLLON), RTD projekt v 5. okvirnem programu EU (do 30. 04. 2005)

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 strnjenim slojem katalizatorja, 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 (Mettler Toledo)
- Avtomatizirani sistem za karakterizacijo heterogenih katalizatorjev (Micromeritics, model Autochem II 2920)
- Masni spektrometer (Pfeiffer Vacuum, model Thermostar)

- Determination of electrochemical and mechanical properties and durability of the new proton conducting polymer membrane for PEM fuel cell, which was developed in collaboration with L02 in the framework of the APOLLON project (5th FP of EU)

- Determination of activity and durability of the new CO-tolerant anode catalysts for PEM fuel cells in collaboration with L10 in the framework of the APOLLON project (5th FP of EU)

COLLABORATION WITH INDUSTRIAL PARTNERS

- Renault, Paris, France, Partnership: Synthesis of proton conducting membranes for high temperature (till 30. 07. 2005), PEMFC (2001 - 2004)

INTERNATIONAL COLLABORATION

- »Waste water treatment by catalytic oxidation contactor« (WATERCATOX), RTD Project in 5th EU Framework Program
- »Advanced PEM Fuel Cells« (APOLLON), RTD Project in 5th EU Framework Program (till 30. 04. 2005)

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 reaction analysis system (Mettler Toledo)
- Automated system for heterogeneous catalysts characterization (Micromeritics, model Autochem II 2920)

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- M. Vospernik: "Snovni transport in kemijska reakcija v trifaznem membranskem reaktorju", doktorsko delo, mentor: A. Pintar
- A. Premrl: "Študij kristalizacije aktivne farmacevtske učinkovine omeprazol", magistrsko delo, mentor: J. Levec.

- Mass spectrometer (Pfeiffer Vacuum, model Thermostar)

EDUCATION AND IMPORTANT VISITS

- M. Vospernik: "Mass transport and chemical reaction in the three-phase membrane reactor"; doctoral thesis, mentor: A. Pintar
- A. Premrl: "Crystallization study of active pharmaceutical ingredient omeprazol"; M.Sc. thesis, mentor: J. Levec

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

Andrej Šonc



PODROČJA DEJAVNOSTI

Razvoj procesov

- Raziskave in razvoj tehnično pomembnih proizvodnih procesov, sodobnih separacijskih operacij, postopkov varstva okolja za kemijsko in procesno industrijo, pristopi k trajnostnemu industrijskemu razvoju
- Povečevanje postopkov iz laboratorijskega v pilotno in polindustrijsko merilo, izvajanje pilotnih poskusov, materialno-energetsko bilanciranje in modeliranje procesov
- Modeliranje in optimiranje delovanja posameznih procesnih elementov in naprav, odpravljanje ozkih grl procesov, zapiranje tehnoloških krogov procesov; izdelava tehnoloških podlag za nove ali inovirane procese
- Merjenje in modeliranje nekaterih termodinamskih ravnotežij večfaznih in večkomponentnih sistemov v širšem obsegu termodinamskih pogojev PTC (tekoče-tekoče, tekoče-parno, tekoče-trdno)

Čiste tehnologije

- Razvoj in integracija preventivnih ukrepov

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 / systems in broad range of thermodynamic conditions and their modelling by means of statistical methods
- Integration of pollution prevention and environmental protection measures in new or existing industrial processes, development of reclamation processes for various 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 hazardous wastes in order to minimise their quantity or hazardness

varstva okolja v industrijske procese; uvajanje principov *čistejše proizvodnje* v industrijsko prakso; izdelava ocen skladnosti proizvodnih procesov z *BAT* tehnologijami po direktivi *IPPC*

- 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

- Izdelava celovitih poročil o vplivih proizvodnih in drugih procesov na okolje (pooblastilo Ministrstva za okolje in prostor (MOP))
- Izdelava načrtov za gospodarjenje z odpadki in ocen o ravnanju z odpadki (pooblastilo MOP)
- Sodelovanje v presojah sistemov za ravnanje z okoljem po ISO 14000 in EMAS (sodelovanje s SIQ)
- Recenzije in revizije razvojnih, predinvesticijskih in ekoloških projektov (pooblastilo MOP)

Servisna dejavnost

- Izvajanje pilotnih poskusov kemijskih sintez in separacij večkomponentnih / večfaznih snovnih sistemov
- Merjenje izbranih fizikalno - kemijskih lastnosti čistih snovi, mešanic in materialov
- Laboratorijska / pilotna proizvodnja specialnih kemičnih izdelkov
- Regeneracija posebno čistih laboratorijskih in procesnih topil (dovoljenje MOP)

BIBLIOGRAFIJA

- 1 izvorni znanstveni članek
- 1 drugi članek in sestavek
- 7 objavljenih znanstvenih prispevkov na konferencah
- 2 objavljena strokovna prispevka na konferencah

- National inventories and balances of critical environmental contaminants, wastes and emissions; related 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

- 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)

BIBLIOGRAPHY

- 1 Original Scientific Articles
- 1 Other Article or Component Part
- 7 Published Scientific Conference Contributions
- 2 Published Professional Conference Contributions
- 2 Published Scientific Conference Contribution Abstracts
- 2 Unpublished Conference Contributions
- 2 Final Research Reports
- 10 Treatises, Preliminary Studies, Studies
- 2 Expertises, Arbitration Decisions
- 2 Undergraduate Theses
- 1 Master's Thesis
- 2 Journal Editorships

RESULTS IN 2005

- Upgrade and update of the national information system on waste generation: data

- 2 objavljena povzetka znanstvenih prispevkov na konferencah
- 2 prispevka na konferencah brez natisa
- 2 končni poročili o rezultatih raziskav
- 10 elaboratov, predštudij, študij
- 2 izvedenski mnenji, arbitražni odločbi
- 2 diplomi
- 1 magisterij
- 2 uredništvi revij

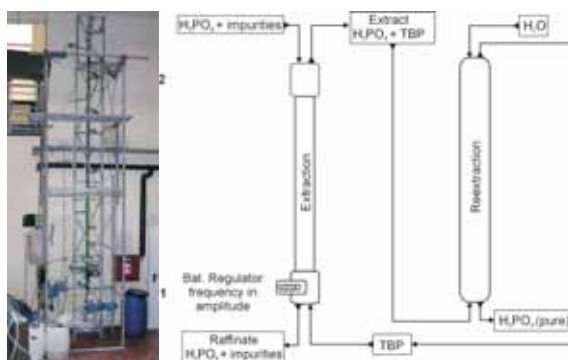
DOSEŽKI V LETU 2005

- Dogradnja državnega informacijskega sistema za področje odpadkov in izdelava nacionalnih bilanc komunalnih, gradbenih, nenevarnih in nevarnih odpadkov za leto 2004, s časovno vrsto od leta 1999, po dejavnostih povzročiteljev, kataloških vrstah odpadkov in načinih ravnanja
- Dokončanje nacionalne bilance emisij hlapnih organskih snovi iz industrije, določitev ukrepov za doseg predpisanega zmanjšanja emisij, ocena stroškov, ocena poteka zmanjševanja emisij do leta 2020
- Izdelava katastra divjih odlagališč odpadkov in predloga prednostne sanacije vodozbirnega območja Jarški brod; 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
- Vključitev v integrirani EU projekt 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); sodelovali bomo v podprojektu SP4 »Production of Discrete Oxigenated Target Compounds« pri identifikaciji optimalnih separacijskih strategij in tehnologij ter razvoju separacijskih tehnologij za izolacijo posameznih frakcij in / ali diskretnih komponent
- 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
- National inventory and information system on the industrial emission of volatile organic compounds, distribution of emissions between industrial sectors, measures identification for reduction of the excess emissions, cost estimation, prediction of emission reduction by implementing various measures till 2020
- Site inspection, environmental risk assessment and remediation planning of: a) water collection area Jarški brod for Ljubljana city water supply, due to illegal dumping of waste; b) abundant industrial site of an old zinc metallurgical plant in Celje, related to its further (public) use
- Participation in preparation of the proposal for European integral EU project BIOCOUP, Module Energy-3 (accepted for financing in the year 2006 onwards); with the title: "Co-processing of upgraded bio-liquids in standard refinery units" on 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
- Research cooperation with Bayer Technology Services Leverkusen, Germany on high pressure technology for determination of thermophysical properties of materials; the beginning of the construction of high-pressure view-cell
- Cooperation with University of Erlangen, Germany on the field of the formation of microparticles by SCF-GAS technique and study of the drug release
- Participation in the Centre of Excellence (co-

- Pogodba o sodelovanju s firmo Bayer Technology Services Leverkusen, Nemčija, na področju visokotlačnih tehnologij za določanje termofizikalnih lastnosti materialov; pričetek izgradnje visokotlačne celice za merjenje faznih ravnotežij
 - Sodelovanje z Univerzo Erlangen, Nemčija, na področju tvorbe mikrodelcev v farmacevtske namene z uporabo SCF-GAS tehnike ter študija sproščanja zdravilnih učinkovin
 - Izdelava systemske dokumentacije in vpeljava sistema za zagotavljanje kvalitete preskusov karakterizacije odpadkov po standardu SIST EN ISO 17025 v naš laboratorij, akreditacijska listina št. SA-L075 pridobljena decembra 2005
 - Izvajanje programa razvoja čistih tehnologij za različne kemične proizvode v okviru centra odličnosti Ekološke tehnologije (nosilec IJS), npr. predelava tehnične fosforne kisline v čisto kislino oz. njene soli z uporabo nove generacije ekstraktantov
 - Zaključek dela v okviru slovenskega tekstilnega grozda na programih vzpostavljanja ekološke komponente trajnostnega razvoja varstva okolja v tekstilni industriji (preprečevanje onesnaževanja, ločevanje in recikliranje odpadkov, čiščenje in recikliranje odpadnih vod, obdelava emisij v zrak)
- ordinator Jo'ef 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
 - Completion of participation in the R&D programme of the slovene textile cluster, aiming towards introduction of sustainable development measures into textile-industry production processes (emission prevention, waste minimisation/recycling, waste treatment and disposal).
 - Accreditation of the laboratory by the National Accreditation Agency for testing of waste and other materials according to SIST EN ISO/IEC 17025
 - Organisation of the 47th Working party meeting on Distillation, Extraction and Adsorption of the European Federation of Chemical Engineering, Ljubljana, Slovenia; September 21. - 23. 2005

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Pilot-plant experiments, process modelling and optimization (non-catalytic chemical syntheses, component/phase separation, mixing



SLIKA 1:
Quickfit pulzirajoča kolona s perforiranimi ploščami v študiji ekstrakcije fosforne kisline s tributilfosfatom

FIGURE 1:
Quickfit pulsed column with perforated plates used in solvent extraction of phosphoric acid by tri-butyl-phosphate

- Pridobitev pooblastil Ministrstva za okolje in prostor za: i) izdelavo ocen odpadkov po pravilniku o ravnanju z odpadki, ii) okoljsko izvedenstvo po Zakonu o varstvu okolja, in iii) za presojo okoljskega ravnanja podjetij po sistemu EMAS (zadnje dvoje *ad personam* - vodja laboratorija), iv) za izvajanje regeneracije laboratorijskih in drugih ekstra čistih kemikalij
- Organizacija (s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani) 47. srečanja delovne skupine za ekstrakcijo, destilacijo in absorpcijo Evropske federacije kemijskega inženirstva EFCE, Ljubljana, 21. – 23. 9. 2005

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

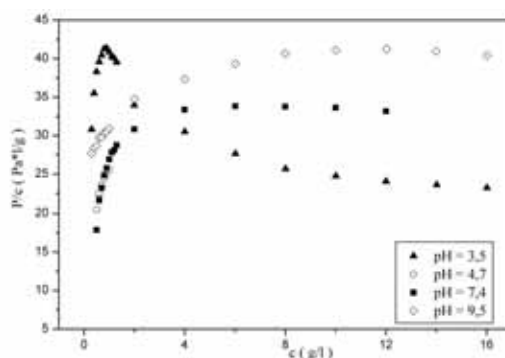
- TKI Hrastnik d.d., Hrastnik
- Belinka – Perkemija d.o.o., Ljubljana
- Lek d.d., Ljubljana
- Agencija RS za okolje, Ministrstvo za okolje in prostor
- Vitiva d.o.o., Markovci
- Regionalna razvojna agencija Celje, d.o.o., Celje

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 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 modelling 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.)



SLIKA 2:
Reduciran ozmotski tlak BSA v puferni raztopini pri pH 3,5 – 9,5 in 298,15 K

FIGURE 2:
Reduced osmotic pressure of BSA in buffer solution at pH 3,5 – 9,5 and 298,15 K

POMEMBNI INŠTRUMENTI 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+, FIX, PARAGON, PROCEDE ...)

IZOBRAŽEVANJE

Mentorstva:

- 1 magistrsko delo
- 2 diplomski deli

Habilitacije in dejavnosti:

- V. Grilc: izr. prof. za področje kemijsko in ekološko inženirstvo (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani).

Poučevanje: Gospodarjenje z odpadnimi snovmi (Fakulteta za gradbeništvo in geodezijo Univerza v Ljubljani – univerzitetni študij vodarstva in komunalnega inženirstva); Ravnanje z odpadki (Interfakultetni podiplomski študij varstva okolja, Univerza v Ljubljani); MBA Studies in Sustainable industrial development - Clean Technology Management, ICPE, Ljubljana; Funkcionalno izobraževanje ob delu za področje komunalnih dejavnosti (Agencija za Management, Ljubljana).

- L. Fele Žilnik: znanstvena sodelavka za področje kemijsko inženirstvo (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani).

Poučevanje: gostujoča predavateljica za del predmeta Termodifuzijske operacije (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani).

EDUCATION

Supervision of student projects:

- 1 MSc project
- 2 BSc projects

Assignments:

- V. Grilc: associate professor in chemical / environmental engineering
- L. Fele Žilnik: research fellow in chemical engineering (both at University of Ljubljana, Faculty for chemistry and chemical technology, lecturing regularly or by invitation on various under- and postgraduate courses in chemical, environmental and civil engineering)

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. Simona Golič Grdadolnik (delno / partly)
Dr. Iztok Jože Košir (delno / partly)
Dr. Gregor Mali (delno / partly)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

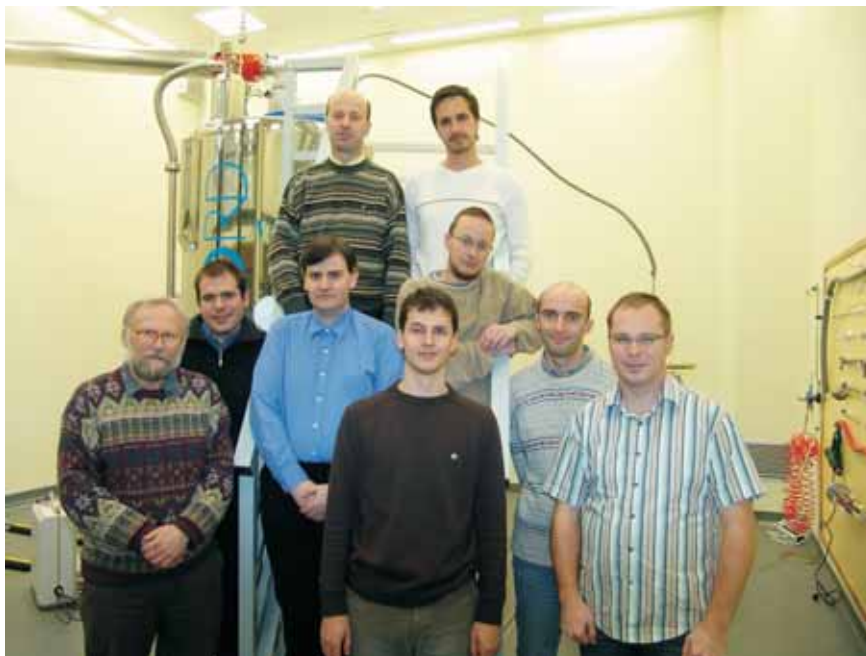
Mirko Cevc
Miha Plevnik (do / until 1. 7. 2005)
Primož Šket

TEHNIČNO OSEBJE / TECHNICAL STAFF

Aleksandar Gačeša
Damjan Makuc
Maja Mirič (polovični čas - od septembra / part
time – since september)

PRIPRAVNIKA / TRAINEES

Gregor Ilc
Peter Podbevšek



SLIKA 1:

Sodelavci NMR centra oz. skupine dr. Plavca pred novim, modernim 800 MHz NMR spektrometrom, ki je začel z obratovanjem v letu 2005.

PODROČJA DEJAVNOSTI

V program delovanja NMR centra za leto 2005 so bile vključene NMR meritve in raziskave za vse uporabnike, ki so 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. Robert Blinc (Institut Jožef Stefan - predsednik), dr. Darko Kocjan (Lek d.d., Ljubljana - namestnik predsednika), dr. Rok Zupet (Krka d.d., Novo mesto), prof. dr. Venčeslav Kaučič (Kemijski inštitut (KI)), dr. Jurka Kidrič (KI), prof. dr. Dani Kikelj (Fakulteta za farmacijo, Univerza v Ljubljani), dr. Mitja Kocjančič (Kmetijski inštitut Slovenije), prof. dr. Branko Stanovnik (Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani), dr. Zoran Šušterič (Sava d.d., Kranj) in dr. Miloš Komac (Ministrstvo za visoko šolstvo, znanost in tehnologijo).

FIGURE 1:

Researchers of NMR centre and members of the Dr. Plavec's group in front of the new, modern 800 MHz NMR spectrometer, which was installed in 2005.

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 2005 included NMR measurements and studies 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. Robert. Blinc (IJS, Ljubljana, Slovenia - president), Dr. Darko Kocjan (Lek d.d., Ljubljana, Slovenia, - vice-president), Dr. Rok

Program dela NMR centra za leto 2005 je obravnaval in potrdil Programski svet NMR centra. V letu 2005 je delo NMR centra potekalo v okviru 61 programov in projektov. Raziskave v okviru NMR centra so v letu 2005 izvajali raziskovalci naslednjih domačih institucij, ki so soustanoviteljice in sovlagateljice v nakup instrumentov NMR centra: Kemijski inštitut (KI); Institut Jožef Stefan; Fakulteta za farmacijo, Univerza v Ljubljani; Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani in Kmetijski inštitut Slovenije. V zadnjih nekaj letih smo sodelovanje NMR centra na KI razširili na uporabnike Narodne in univerzitetne knjižnice, 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 d.d., Ljubljana; Krka d.d., Novo mesto in Helios d.d., Domžale, jih kot sovlagatelj pri nakupu osnovne opreme NMR centra uporabljajo pri rutinski analitiki in v okviru svojega raziskovalno-razvojnega dela. V letu 2005 so instrumente v okviru NMR centra na KI uporabljali tudi raziskovalci iz podjetij Fenolit d.d., Borovnica; Pliva d.d., Zagreb, Hrvaška; Austrian Research Center, Seibersdorf, Avstrija in Donau Chemie, Brückl, Avstrija. Nekaj meritev smo opravili za potrebe sodišča.

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

Zupet (Krka d.d., Novo mesto, Slovenia), Prof. Dr. Venčeslav Kaučič (National Institute of Chemistry (NIC)), Dr. Jurka Kidrič (NIC), Prof. Dr. Daniel Kikelj (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. Miloš Komac (Ministry of Higher Education, Science and Technology).

In 2005 the cooperation between various research groups and NMR centre at NIC involved 61 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, Ljubljana, Slovenia; Faculty of Pharmacy and Faculty of Chemistry and Chemical Technology, University of Ljubljana 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 and Medicinal Faculty of University of Ljubljana, Slovenia and Polytechnic, 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 2005 NMR centre offered services and help to companies Fenolit d.d., Borovnica, Slovenia; Pliva d.d., Zagreb, Hrvaška; Austrian Research Center, Seibersdorf, Austria and Donau Chemie, Brückl, Austria.

Research activities of NMR centre focused on:

- structure of oligomeric nucleic acids fragments and conformational changes in DNA building blocks upon interaction with metal ions

- 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 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, magistrskih in doktorskih del.
- Leto 2005 je pomembno zaznamovalo dogajanje okoli posodobitve opreme NMR centra z investicijo v nov 800 MHz NMR spektrometer in obnovo obstoječe opreme. Zgradili smo novo stavbo. 800 MHz NMR spektrometer je začel s poskusnim obratovanjem oktobra 2005.

BIBLIOGRAFIJA

- 6 izvirnih znanstvenih člankov
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavatelj)
- 2 objavljena znanstvena prispevka na konferencah
- 14 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 2 predavanja na tujih univerzah
- 1 vabljeni predavatelj na konferenci brez natisa
- 1 diploma
- 2 doktorata

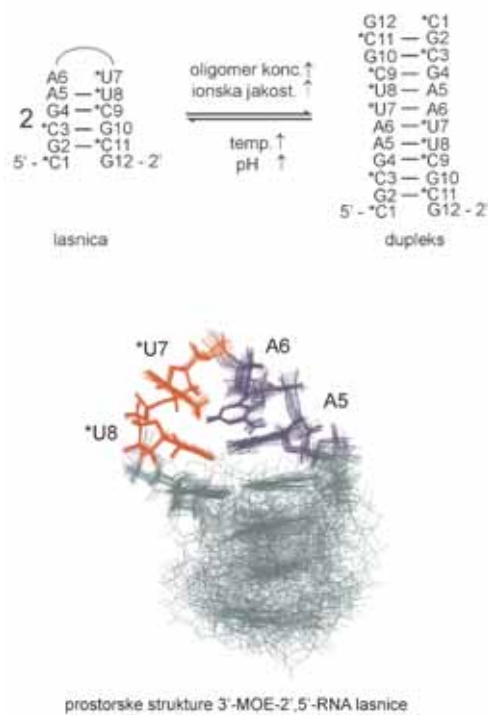
- protein structure and dynamics, protein folding and molecular interactions of peptides with lipopolysaccharides
- ligand-receptor interactions
- structure and dynamics of antibiotics in relation with their biological role
- structure and dynamics of organic molecules, detection and characterization 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.

In 2005 we were largely involved with upgrade of NMR equipment by investment into new 800 MHz spectrometer and upgrade of existing instruments. We have built a new building. New 800 MHz NMR spectrometer has been put into trial operation in October 2005.

BIBLIOGRAPHY

- 6 Original Scientific Articles
- 1 Published Scientific Conference Contribution (Invited Lecture)



SLIKA 2:

Modifikacije nukleinskih kislin vodijo do novih lastnosti, ki so zelo pomembne za uporabnost nukleinskih kislin v medicini, biologiji in biotehnologiji. Poznavanje prostorskih struktur nukleinskih kislin je ključnega pomena za razumevanje njihovih bioloških funkcij. Z uporabo NMR spektroskopije in molekulske dinamskih izračunov smo določili prostorsko strukturo lasnice 3'-MOE-2',5'-RNA oligonukleotida. Ta je v raztopini udeležen v ravnotežju med strukturama lasnice in dvojne vijačnice, ki je odvisno od koncentracije oligonukleotida, koncentracije soli, temperature in pH raztopine. Kot prvi v literaturi smo opisali prostorsko strukturo lasnice, ki ima le 2',5'-fosfodiesterne vezi. Zanka 2',5'-povezane lasnice je nov strukturni motiv in je zelo dobro strukturno določena. Naši rezultati kažejo na velik vpliv sprememb sladkorno-fosfatnega skeleta na tvorbo struktur nukleinskih kislin. Avtorji M. Plevnik, Z. Gdaniec in J. Plavec so rezultate objavili v članku z naslovom "Solution structure of a modified 2',5'-linked RNA hairpin involved in an equilibrium with duplex", ki je bil objavljen v reviji *Nucleic Acids Res.* (2005, 33, 1749-1759).

FIGURE 2:

Modifications of nucleic acids bestow new properties and functions that can be useful for practical application of nucleic acids to medicine, biology and biotechnology. Knowledge of three-dimensional structures of nucleic acids is essential for understanding of their biological functions. Using NMR spectroscopy and restrained molecular dynamics calculations we have determined the solution structure of 3'-MOE-2',5'-RNA hairpin. 3'-MOE-2',5'-RNA oligonucleotide is involved in structural equilibrium between hairpin and duplex structures, that is highly influenced by oligonucleotide concentration, salt concentration, temperature and pH. Our report is the first solution structure of a fully 2',5'-linked RNA hairpin, which displays a unique structural motif and well-defined loop. Our results illustrate the tremendous effect of modifications in the sugar-phosphate backbone on the folding of nucleic acids. Results of M. Plevnik, Z. Gdaniec and J. Plavec were published in the manuscript entitled "Solution structure of a modified 2',5'-linked RNA hairpin involved in an equilibrium with duplex", which appeared in *Nucleic Acids Res.* (2005, 33, 1749-1759).

GLAVNI DOSEŽKI V LETU 2005

Inštalirali smo nov 800 MHz NMR spektrometer, ki med drugim omogoča večjo občutljivost in ločljivost glede na obstoječo opremo.

V teku je projekt Center odličnosti, pri katerem sodelujemo sodelavci KI, 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,
4. karakterizacija rekombinantnih proteinov in bioloških makromolekul v raztopini in
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 preko 30 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 KI ali na drugih inštitutih in fakultetah. Dosežki sodelovanja med NMR centrom in slovensko industrijo so javno znani le preko uspešnega poslovnega rezultata posameznega podjetja.

- 2 Published Scientific Conference Contributions
- 14 Published Scientific Conference Contribution Abstracts
- 2 Invited Lectures at Foreign Universities
- 1 Unpublished Invited Conference Lecture
- 1 Undergraduate Thesis
- 2 Doctoral Dissertations

IMPORTANT ACHIEVEMENTS IN 2005

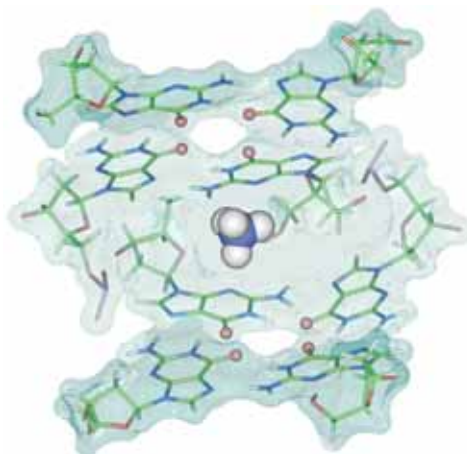
Project Centre of Excellence prepared jointly by researchers from NIC, Lek and Krka has been approved.

The new 800 MHz NMR spectrometer has been installed. We value among other aspects its higher sensitivity and resolution.

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 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 30 publications in journals with international peer review evaluation procedure (complete list is available on NMR center's home-



SLIKA 3:

Vpogled med dve G-kvartetni ravnini, ki sestavljata G-kvadrupleksno strukturo (na levi). V središču vsakega G-kvarteta so prostorsko blizu štirje O6 karbonilni kisikovi atomi (na levi sliki označeni z rdečimi kroglicami), katerih nevezni elektronski pari sodelujejo pri koordinaciji kationov, ki so nujno potrebni za nastanek G-kvadrupleksne strukture. V konkretnem primeru je amonijev ion koordiniran z osmimi O6 karbonilnimi kisikovimi atomi, ki pripadajo dvema G-kvartetoma. Kationi znotraj takšnih struktur ne mirujejo, ampak se izmenjujejo preko odprtih v G-kvartetnih ravninah. Slika je del študije, kjer so P. Šket, M. Črnugelj in J. Plavec pokazali, da se znotraj dimernega G-kvadrupleksa, ki ga tvori oligonukleotidno zaporedje bogato z gvanini $d(G_3T_4G_4)$, nahajata dve vezavni mesti za katione. V nadaljevanju so uspeli dokazati obliko G-kvadrupleksa $d(G_3T_4G_4)_2$, ki vsebuje K^+ in $^{15}NH_4^+$ ion in predstavlja vmesno stanje v prehodu iz dvo- $^{15}NH_4^+$ v dvo- K^+ obliko. Korelacijski signali v ROESY spektru med amonijevimi ioni in imino protoni gvaninov, ki je prikazan na desni so dali informacijo o položaju amonijevega iona znotraj te strukture. Rezultati te študije so bili objavljeni v članku z naslovom "Identification of mixed di-cation forms of G-quadruplex in solution" v reviji *Nucleic Acids Res.* (2005, 33, 3691-3697).

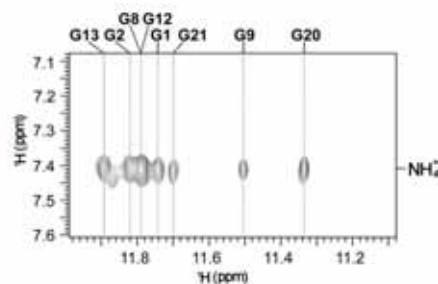


FIGURE 3:

Detailed view into the structure of a G-quadruplex showing two G-quartet planes (on the left side). There are four O6 carbonyl oxygen atoms (marked as red balls) in the middle of each G-quartet, which are involved in coordination with cations that are essential for the formation of G-quadruplex structures. Ammonium ion in the figure is coordinated with eight O6 carbonyl oxygen atoms belonging to two neighbouring G-quartet planes. Cations found inside G-quadruplex structures are undergoing fast and complex motion through the opening in each G-quartet plane. Figure is a part of a study in which P. Šket, M. Črnugelj and J. Plavec have shown that dimeric G-quadruplex structure adopted by guanine rich sequence $d(G_3T_4G_4)$ exhibits two cation binding sites. Furthermore, they experimentally demonstrated the existence of the mixed form of $d(G_3T_4G_4)_2$ containing one K^+ and one $^{15}NH_4^+$ ion inside the G-quadruplex core that represents intermediate in the conversion of di- $^{15}NH_4^+$ into di- K^+ form. Cross-peaks in ROESY spectrum between ammonium ions and neighbouring guanine imino protons shown on the right were used to localize ammonium ions inside the mixed di-cation structure. The results of the study were published in the manuscript entitled "Identification of mixed di-cation forms of G-quadruplex in solution" in *Nucleic Acids Res.* (2005, 33, 3691-3697).

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 s 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 so v letu 2005 bili:

- Fenolit d.d., Borovnica
- Pliva d.d., Zagreb, Hrvaška
- Austrian Research Center, Seibersdorf, Avstrija
- Donau Chemie, Brückl, Avstrija

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 Unity Inova 600
- Varian Unity Inova 300
- Varian Unity Inova 300

IZOBRAŽEVANJE

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, magistrskih in doktoratov.

V preteklem letu sta svoji doktorski dizertaciji, ki sta ju v celoti opravila v okviru NMR centra pod mentorstvom J. Plavca uspešno zagovarjala M. Plevnik in P. Šket.

- M. Plevnik je svoje podiplomsko izobraževanje zaključil z doktorsko dizertacijo z naslovom "Strukturne raziskave predorganizacije

page 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:

- Lek d.d., Ljubljana, Slovenia
- Krka d.d., Novo mesto, Slovenia
- Helios d.d., Domžale, Slovenia

The other users of our services and expertise in 2005 were:

- Fenolit d.d., Borovnica, Slovenia
- Pliva d.d., Zagreb, Croatia
- Austrian Research Centre, Seibersdorf, Austria
- Donau Chemie, Brückl, Austria

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 Unity Inova 600
- Varian Unity Inova 300
- Varian Unity Inova 300

prostorskih struktur oligomernih nukleinskih kislin". S svojo doktorsko dizertacijo je kandidiral na razpis 35. Krkinih nagrad in je bil izmed 47 nagrajencev izbran med pet dobitnikov nagrad za posebne dosežke.

- P. Šket je doktoriral s tezo z naslovom "NMR študije vezave kovinskih ionov znotraj G-kvadrupleksnih struktur DNK".
- V skupini vodje NMR centra je leta 2005 svoje dodiplomsko izobraževanje zaključil P. Podbevšek z diplomskim delom z naslovom "Študij vezave amonijevih ionov znotraj G-kvadrupleksa $d(G_4(T_4G_4)_3)$ ".

EDUCATION

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.

The following young researchers have successfully completed their education in 2005 by thesis work performed under the supervision of J. Plavec:

- M. Plevnik with Ph.D. thesis entitled "Structural Studies of Preorganization of 3D Structures of Oligomeric Nucleic Acids"
- P. Šket with Ph.D. thesis entitled "NMR Studies of cation binding within G-quadruplex DNA structures"
- P. Podbevšek with B.Sc. thesis entitled "Studies on Ammonium Ion Binding within the $d(G_4(T_4G_4)_3)$ G-quadruplex"

M. Plevnik has applied to the 35th Krka Awards and was amongst 47 prize winners chosen to be among five awards for extraordinary achievements.

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 Ciglaric (od / since 2. 12. 2005)

Katarina Jankovič

Adolf Krašna

Darija Lorber (začasno odsotna – porodniški dopust / temporary absence - maternity leave)

Tanja Maver

Katja Rožmanc Babnik

Barbara Lečnik Spaić



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 bioanaliznih 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 2005

CVTA sledi naraščajočim potrebam slovenske in tuje farmacevtske industrije po analitski podpori

ACTIVITIES

CVTA designs and perform the following activities related to medicines and food:

- development of HPLC, GC, TLC, dissolution testing and other analytical procedures
- analyses and analytical studies for quality control of products, and 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 2005

CVTA follows the increasing needs of pharmaceutical industry for analytical support to their R&D and production projects, combined with sharpening requirements of quality standards. In principle it represents a novel organizational model, which was in 2005 successfully further developed and adjusted to the needs of indus-

razvojnim in proizvodnim projektom ob zaostrovanju kakovostnih zahtev za izvajanje takšnih del. Konceptualno predstavlja novi model izvajanja nalog za potrebe industrije, ki smo ga v l. 2005 nadalje uspešno razvijali ter organizacijsko in vsebinsko prilagajali potrebam naročnikov. Tako smo razširili spekter tehnik plinske kromatografije ter uvedli tehnike za določanje hitrosti raztapljanja učinkovin iz končnih farmacevtskih izdelkov. Delo v CVTA poteka ob strokovni podpori Laboratorija za prehrabeno kemijo (L06).

V l. 2005 smo za slovensko farmacevtsko industrijo izvedli:

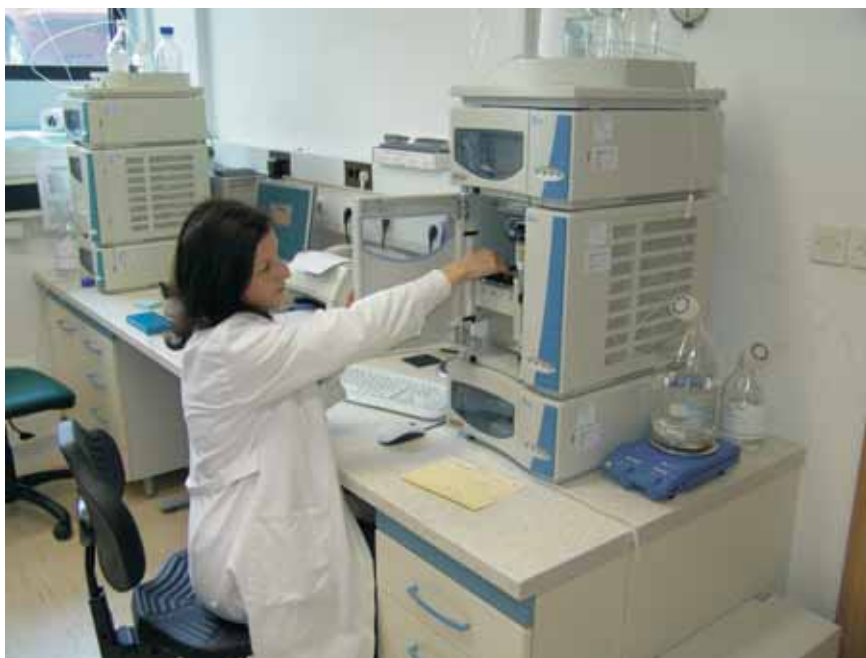
- razvoj 8 analitskih postopkov
- validacijo 67 HPLC, GC in TLC analitskih postopkov
- analize za validacijo več proizvodnih tehnologij
- analize za validacije več tehnologij čiščenja proizvodne opreme

trial partners. In this respect we have broadened a spectrum of gas chromatography techniques, and introduced techniques of dissolution testing important for evaluation of finished dosage forms. All the activities were performed in tight collaboration with L06, which offered professional support of its experts to CVTA.

Crucial achievements in the year 2005 are:

- Development of 8 analytical methods
- Validation of 67 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 550 samples of pharmaceutical finished dosage forms.

All activities were performed according to GLP and/or GMP standards.



SLIKA:
Delo na HPLC sistemu

FIGURE:
Working on HPLC system

- analize v okviru stabilitetnih študij za več preparatov
- analize rezidualnih topil v ca. 550 vzorcih različnih preparatov.

Vsa dela so bila izvedena v skladu s standardi dobre laboratorijske oz. dobre proizvodne prakse.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

CVTA je v skladu s cilji vse prihodke v l. 2005 ustvaril z delom za farmacevtsko industrijo, zlasti z družbama Lek d.d., Ljubljana in Krka d.d., Novo mesto.

POMEMBNI INSTRUMENTI 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).

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

According to the goals CVTA has earned all incomes by activities for industrial partners, particularly Lek d.d., Ljubljana, Slovenia - the member of Sandoz company, and Krka d.d., Novo mesto, Slovenia.

MAJOR EQUIPMENT

Several HPLC systems, two GC and TLC system, as well as 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

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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L02

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L03

Laboratorij za kemometrijo

Laboratory of Chemometrics

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Uredništva / Editorships

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L04

Laboratorij za analizno kemijo

Analytical Chemistry Laboratory

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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L05

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Laboratory for Chemistry, Biology and Technology of Water

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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

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L07

Laboratorij za polimerno kemijo in tehnologijo

Laboratory for Polymer Chemistry and Technology

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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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Uredništva / Editorships

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L09

Laboratorij za anorgansko kemijo in tehnologijo

Laboratory for Inorganic Chemistry and Technology

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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Mentorstva / Mentorships

15. RISTIĆ, Alenka, Kaučič, Venčeslav (mentor). Sinteza molekulskih sit z železoaluminofosfatnim ogrodjem : doktorska disertacija. Ljubljana: [A. Ristić], 2005. [6] + 88 f., graf. prikazi, tabele. [COBISS.SI-ID 3283226]

Uredništva / Editorships

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17. International journal of molecular sciences. Kaučič, Venčeslav (član uredniškega odbora 2001-). Basel: MDPI Center. ISSN 1422-0067. [COBISS.SI-ID 2779162]
18. Microporous and mesoporous materials. Kaučič, Venčeslav (član uredniškega odbora 2003-). Amsterdam (etc.): Elsevier, 1998-. ISSN 1387-1811. [COBISS.SI-ID 1595162]

L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

1. BELE, Marjan, DMITRAŠINOVIĆ, Djordje, PLANINŠEK, Odon, SALOBIR, Mateja, SRČIČ, Stanko, GABERŠČEK, Miran, JAMNIK, Janko. Silica coatings on clarithromycin. *Int. J. Pharm.*, 2005, vol. 291, no. 1/2, str. 149-153. [COBISS.SI-ID 3204378]
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9. STRMČNIK, Dušan, GABERŠČEK, Miran, HOČEVAR, Stanko, JAMNIK, Janko. The effect of halide ion impurities and Nafion on electrooxidation of CO on platinum. *Solid State Ion.*, 2005, vol. 176, no. 19/22, str. 1759-1763. [COBISS.SI-ID 3317274]
10. VRATNICA, Zoran, VUJOŠEVIĆ, Danijela, BELE, Marjan, DRENIK, Aleksander, VESEL, Alenka, CVELBAR, Uroš, MOZETIČ, Miran. Preiskave bakterij s sodobnim vrstičnim elektronskim mikroskopom. *Vakuumist*, 2005, let. 25, št. 1-2, str. 20-23. [COBISS.SI-ID 19220007]
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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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15. STAKNE, Kristina, KUREČIČ, Manja, GREGOR-SVETEC, Diana, BELE, Marjan, KREŽE, Tatjana, SFILIGOJ-SMOLE, Majda. Properties of ionexchange PP nanocomposite fibres. V: MAJCEN LE MARECHAL, Alenka (ur.), STJEPANOVIČ, Zoran (ur.), KOKOL, Vanja (ur.), ŽUNIČ-LOJEN, Darja (ur.), FAKIN, Darinka (ur.), FUŽIR BAUER, Gabrijela (ur.), ZIMŠEK, Danijel (ur.), KRIŽANEC, Boštjan (ur.), VOLMAJER, Julija (ur.), VONČINA, Bojana (ur.). 5th World Textile Conference AUTEX 2005, 27-29 June 2005, Portorož, Slovenia. Proceedings. Maribor: Faculty of Mechanical Engineering, Department of Textiles, 2005, str. 244-248. [COBISS.SI-ID 1493872]

16. VAVPOTIČ, Marko, BELE, Marjan, ŠTIBLAR-MARTINČIČ, Draga, BALAŽIČ, Jože. In vitro decalcification of human dentin investigated by field emission scanning electron microscopy : [poster]. V: ČEH, Miran (ur.), DRAŽIČ, Goran (ur.), FIDLER, Sanja (ur.). 7th Multinational Congress on Microscopy, June 26-30, 2005, Portorož, Slovenia. Proceedings. Ljubljana: Slovene Society for Microscopy: Department for Nanostructured Materials, "Jožef Stefan" Institute, 2005, str. 527-528. [COBISS.SI-ID 3309594]

Patenti in patentne prijave / Patents and Patent Applications

17. STAKNE, Kristina, SFILIGOJ-SMOLE, Majda, STANA-KLEINSCHEK, Karin, LOBNIK, Aleksandra, BELE, Marjan, JAMNIK, Janko. Metoda za modifikacijo raznovrstnih vlaken z nanonanosi : prijava patenta P-200500210, datum vložitve prijave 19.7.2005. Ljubljana: Urad Republike Slovenije za intelektualno lastnino, 2005. 7 f. [COBISS.SI-ID 9804566]

Mentorstva / Mentorships

18. MOŠKON, Jože, Bešter-Rogač, Marija (mentor), Gaberšček, Miran (komentor). Prevodne ogljikove prevleke na izbranih modelnih substratih : diplomsko delo. Ljubljana: [J. Moškon], 2005. 104 f., ilustr. [COBISS.SI-ID 27193349]
19. ZORAN, Alenka, Planinšek, Odon (mentor), Bele, Marjan (komentor). Vpliv velikosti specifične površine in dodatka površinsko aktivnih snovi na raztapljanje naproksena = The influence of specific surface area and surface active agents on the naproxen dissolution rate : diplomska naloga, (Fakulteta za farmacijo, Ljubljana, Diplomske naloge, 1990). Ljubljana: [Zoran, A.], 2005. 55 f., ilustr. [COBISS.SI-ID 1715313]
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Uredništva / Editorships

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Intervjuji / Interviews

22. VENTURINI, Peter, Koren, Ksenija (oseba, ki intervjuva). Bolj kot prodajanja izdelkov si želimo prodajanja domačega znanja : znanstvenik, ki je delal v gospodarstvu, in direktor Kemijskega inštituta dr. Peter Venturini : o tem, kje škripa, da slovenska znanost in gospodarstvo ne sodelujeta dovolj, pa tudi o dobrih primerih, ki bi morali postati zgled ostalim znanstvenikom in gospodarstvenikom. Večer (Marib.). [Tiskana izd.], 1. apr. 2005, letn. 61, št. 74, str. 3. [COBISS.SI-ID 3272730]

23. VENTURINI, Peter, Vagaja, Aleksandra (oseba, ki intervjuva). Nanotehnologija je finančno podhranjena : država bi morala ustvariti razmere, v katerih bodo vlaganja v razvoj in raziskave cenejša in bolj zanimiva. *Finance*. [Tiskana izd.], 9. junij 2005, št. 110[2045], str. 24, priloga Nanotehnologija, fotografija avtorja. [COBISS.SI-ID 3318810]

L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation

V celoti objavljeni članki (znanstveni, strokovni, poljudni) / Full Text Articles

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Narejeno v sodelovanju z Medicinsko fakulteto Univerze v Ljubljani /
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

1. ANDRÄ, Jörg, LOHNER, Karl, BLONDELLE, Sylvie E., JERALA, Roman, MORIYON, Ignacio, KOCH, Michel H. J., GARIDEL, Patrick, BRANDENBURG, Klaus. Enhancement of endotoxin neutralization by coupling of a C12-alkyl chain to a lactoferricin-derived peptide. *Biochem. J.*, 2005, vol. 385, part 1, str. 135-143. [COBISS.SI-ID 3182106]
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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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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

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