

Poročilo o delu 2007

Annual report 2007

POROČILO O DELU 2007 / ANNUAL REPORT 2007

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Beseda direktorja

Word of the Director



V poslanstvu se je Kemijski inštitut zavezal znanstveni odličnosti, izobraževanju in dobremu sodelovanju z gospodarstvom, saj želimo pomembno prispevati k izboljševanju kvalitete življenja in ekonomskemu napredku naše družbe.

Za doseganje visokih ciljev je ključno doseganje najvišje svetovne ravni znanja ter ustvarjanje pogojev za ohranitev in pritegnitev najboljših strokovnjakov. Velike investicije, tudi v večjo raziskovalno opremo, ter posodobitve inštituta omogočajo takšne pogoje dela, ki so bolj primerljivi z najuspešnejšimi raziskovalnimi ustanovami po svetu. Dober primer uspešnosti naše usmeritve je Nacionalni center za NMR spektroskopijo visoke ločljivosti, ki omogoča delo na vrhunski infrastrukturi domačim in tujim raziskovalcem iz akademskih in gospodarskih organizacij. Naši znanstveni cilji postajajo s sodobnejšo raziskovalno opremo višji, bolj samozavestno lahko nastopamo tudi v mednarodnem prostoru. V preteklih letih je takšna strategija prispevala k stalnemu dvigu kvalitete znanstvenih publikacij naših raziskovalcev in njihovo večjo odmevnost. Postali smo uspešen

In its mission statement the National Institute of Chemistry has pledged to devote itself to scientific excellence, education and strong cooperation with industry, since it is our goal to make an important contribution to the improvement of the quality of life and economic advancement of our society.

In order to reach such high goals one must strive towards the highest level of science and one must create the conditions necessary to keep and attract the best scientists. Large investments, such as those into research equipment and modernization of the Institute, have allowed us to create working conditions that are more comparable to some of the most successful research institutions in the world. A good example of the success of our current direction is the National Center for High Resolution NMR Spectroscopy, which allows domestic and foreign researchers from academic and industrial organizations access to top-notch infrastructure. With more modern research equipment, our scientific goals have become higher and we are able to conduct ourselves more confidently in the international sphere. Over the past few years

partner in koordinator evropskih in drugih mednarodnih raziskovalnih projektov. Inštitut sodeluje pri organizaciji seminarjev in največjih mednarodnih znanstvenih srečanj. V lanskem letu je zelo odmeval Evropski polimerni kongres v Portorožu s preko 800 udeleženci iz 49 držav. Velika vpetost v mednarodni prostor, ki se kaže v sodelovanjih v skupnih mednarodnih združenjih, projektih in organizaciji mednarodnih znanstvenih srečanj, pa povečuje tudi interes tujih znanstvenikov za raziskovalno delo na Kemijskem inštitutu. Število znanstvenikov na Kemijskem inštitutu, ki prihajajo iz tujine, je zato vse večje.

Kemijski inštitut je zgradil trdna partnerstva z univerzami in gospodarstvom, kar omogoča skupno delo na raziskovalnih projektih in usklajeno investiranje v večjo raziskovalno opremo.

Z univerzami smo zgradili medsebojno zaupanje, ki omogoča odkrite razgovore in boljše sodelovanje. Dobro sodelovanje pa prinese tudi odmevne uspehe. Primer takšnega sodelovanja iz leta 2007 je ponovitev odličnega uspeha študentov na svetovnem tekmovanju iz sintezne biologije, kjer so premagali ekipe iz univerz, ki se na mednarodnih lestvicah kakovosti uvrščajo najvišje. Na Kemijskem inštitutu pa opažamo tudi vse večji interes študentov za raziskovalno delo na naši instituciji za izdelavo tako diplomskih del kot tudi doktorskih disertacij.

Mnogi raziskovalci na Kemijskem inštitutu so usposobljeni in imajo željo za uspešno sodelovanje s podjetji. Nadaljuje se trend hitre rasti sodelovanja z gospodarstvom. Pomembno vlogo pri tem ima dobro urejeno poslovanje inštituta. Ponosni smo, da smo pomembno prispevali k razvoju tehnologij za biološka zdravila v Leku, ki je sedaj med redkimi podjetji v svetu, ki trži zdravila, ki so produkt te zahtevne tehnologije.

V preteklih letih smo se lotili nekaterih dolgoročnih ciljev, ki še niso realizirani. Pomemben cilj Kemijskega inštituta je še

this strategy has contributed to the continuous rise in the quality of scientific publications of our researchers and to their greater visibility. We have become a successful partner and coordinator of European and other international research projects. One of the great successes of the past year was the European Polymer Congress held in Portorož, organized by our Laboratory for Polymer Chemistry and Technology, which had more than 800 participants from 49 countries. Greater involvement in the international sphere, which is shown through the cooperation of groups in international associations, projects and organizations of international scientific meetings, has also increased the interest of foreign scientists in conducting research work at the National Institute of Chemistry. The number of foreign scientists working at NIC is therefore rising.

NIC has built up a strong partnership with universities and the industry, which has allowed joint work on research projects and harmonized investment in larger research equipment.

We have also built up a bank of mutual trust with the university, which allows more open discussions and better cooperation. Better cooperation also brings greater success. An example of this cooperation is the 2007 repeat of the great success at the world competition in synthetic biology, where students from Slovenia overcame competing groups from some of the highest ranking universities in the world. We have also seen an increase in student interest in carrying out undergraduate and graduate research work towards their PhDs at our Institute.

Many researchers at NIC are capable and have the desire to cooperate successfully with industry. The trend towards faster growth in terms of cooperation with industry continues. The smooth operation of the Institute has played an important part in this. We are proud that we have been able to contribute to the development of technology for biological drugs at Lek Pharmaceutical Company, which is one of

aktivnejše vključevanje v izobraževalni sistem in ustanovitev Raziskovalne šole Kemijskega inštituta. Pričakujemo, da v letošnjem letu pridobimo vsa potrebna soglasja in dokončamo proces ustanavljanja šole. Tako bodo raziskovalci Kemijskega inštituta še bolj prispevali k doseganju visoke kvalitete izobraževanja v Sloveniji in pomagali pritegniti ambiciozne dijakinje in dijake v študij naravoslovja in tehnike.

Mnoge obnove in adaptacije na inštitutu so omogočile boljše pogoje za delo in nekoliko omilile prostorsko stisko. Kljub temu je lahko trajnejša rešitev, ki bi omogočila nadaljnji razvoj inštituta tudi v smeri izobraževanja le postavitev novega objekta inštituta. Pomembno je, da so odločitve glede preselitve sprejete čim hitreje.

K odličnim rezultatom Kemijskega inštituta v letu 2007 so prispevali prav vsi sodelavci in partnerji inštituta. Pred Kemijskim inštitutom pa še ostajajo veliki izzivi, ki jih bo mogoče sprejeti le z dobrim sodelovanjem na inštitutu in trdnim partnerstvom navzven.

the rare companies in the world that is marketing drugs that are products of this demanding technology.

In the past few years we have set out some long-term goals, which have not yet been realized. One of the important goals of the Institute has been to be more actively included in the educational system and to establish the Research School of the National Institute of Chemistry. We expect that we will receive the necessary consensus this year and wrap up the process of setting up the school. Thus, the researchers at NIC will contribute even more to creating higher quality education in Slovenia and will help to attract ambitious high school students into the study of the natural sciences and technology.

The many renovations and adaptations at the Institute have created better working conditions and helped to improve the tight space issues. However, the only long-term solution that will truly help the development of the Institute, even in the area of education, will be moving into a new larger building. It is very important that decisions regarding such a move be made as quickly as possible.

All of the employees, students, and partners of the NIC have contributed to the great results achieved by the Institute in 2007. Nevertheless, there are still great challenges awaiting NIC, which can only be faced with strong cooperation within the Institute and solid partners from outside the Institute.



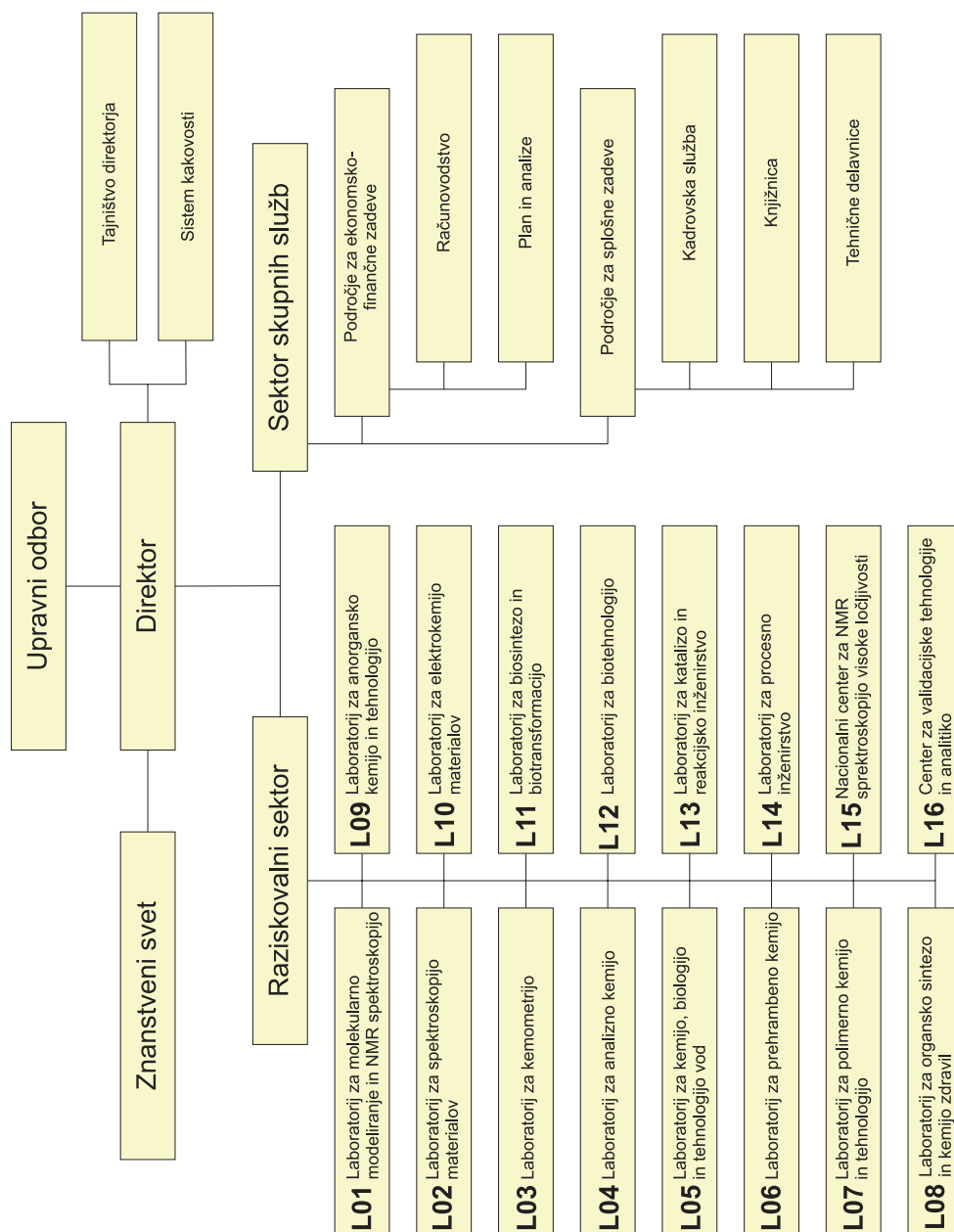
doc. dr. Peter Venturini

Poslanstvo Kemijskega inštituta

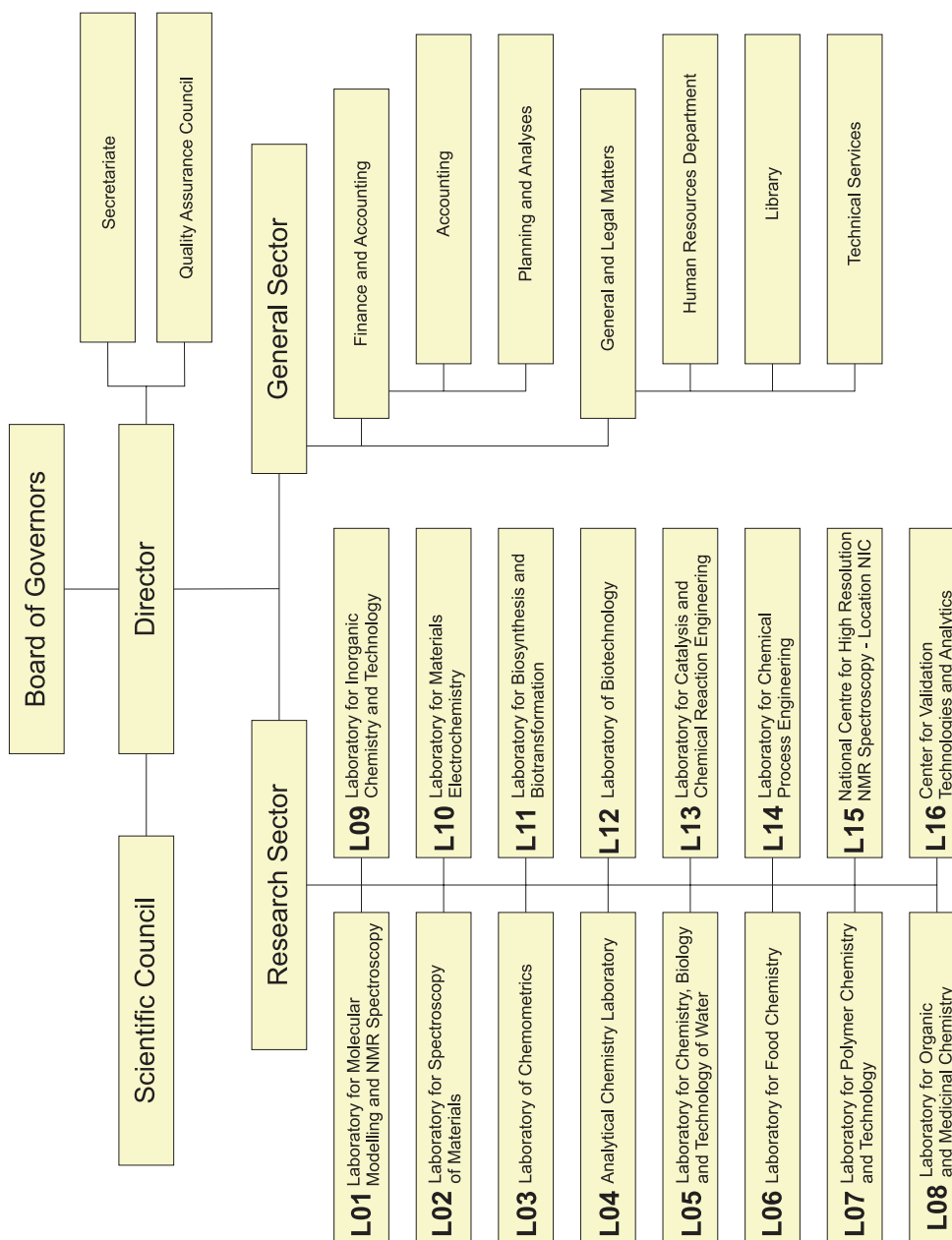
The Mission of the National Institute of Chemistry

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

Organizacijska shema



Organisation Chart



Vodstvo inštituta

Institute Management

VODSTVO / MANAGEMENT

- **Direktor / Director**
doc. dr. Peter VENTURINI
- **Pomočniki direktorja / Assistant directors**
mag. Renata VUGA
mag. Andreja VRAN (do / until 16.12.2007)
Joži ČEŠNOVAR (v.d. pomočnice direktorja, od / since 21.12.2007)
- **Svetovalca direktorja / Councillors to the director**
doc. dr. Janko ŽMITEK
Joži ČEŠNOVAR (od / since 7.5.2007, do / until 21.12.2007)

ČLANI UPRAVNEGA ODBORA / BOARD OF GOVERNORS

- dr. Matej Penca, predsednik / president
- prof. dr. Janez Plavec, podpredsednik / vice-president
- mag. Janko Burgar (od / since 1.2.2007 do / until 20.6.2007)
- dr. Gregor Gomišček
- prof. dr. Roman Jerala
- doc. dr. Andrej Kitanovski (do / until 1.2.2007)
- prof. dr. Tamara Lah
- dr. Brina Ornik
- Bogo Šest
- prof. dr. Tomaž Šolmajer
- doc. dr. Aleš Štrancar (od / since 20.6.2007)

ČLANI ZNANSTVENEGA SVETA / SCIENTIFIC COUNCIL

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

ČASTNI ČLANI / HONORARY MEMBERS

- prof. dr. Igor BELIČ[‡], 19. 12. 1986
- dr. Marta BLINC[‡], 19. 12. 1986
- prof. dr. Bojan DRŽAJ[‡], 19. 12. 1986
- dr. Jože FEGEŠ[‡], 19. 12. 1986
- prof. dr. Vera JOHANIDES[‡], 19. 12. 1986
- prof. dr. Roman MODIČ[‡], 19. 12. 1986
- prof. dr. Tihomir NOVAKOV, 19. 12. 1986
- prof. dr. Robert LAFFERTY, 15. 6. 1994
- prof. dr. Walter STEINER, 15. 6. 1994
- prof. dr. D. Luc MASSART[‡], 8. 3. 1995
- prof. dr. John R. HELLIWELL, 21. 10. 1996
- prof. dr. Joachim MAIER, 17. 4. 1996
- prof. dr. Dušan HADŽI, 9. 10. 2001
- prof. dr. Joseph WANG, 15. 6. 2007
- prof. dr. Milan RANDIĆ, 27. 9. 2007

Finance

PRIHODKI (EUR)

	2007	2006	Struktura 2007 (%)	Indeks 2007/2006
Raziskovalni programi	3.683.356	3.629.904	29	101
Infrastrukturni programi	407.598	418.777	3	97
Raziskovalni projekti	1.196.812	1.129.784	10	106
Ustanoviteljske obveznosti	1.530.986	1.501.269	12	102
Mladi raziskovalci	1.745.867	1.278.041	14	137
Domači trg	2.549.295	2.416.579	20	105
Tuji trg	550.659	413.784	4	133
Drugi prihodki	895.120	914.310	7	98
SKUPAJ PRIHODKI	12.559.695	11.702.447	100	107

ODHODKI (EUR)

	2007	2006	Struktura 2007 (%)	Indeks 2007/2006
Stroški materiala	-1.439.881	-1.357.143	12	106
Stroški storitev	-1.913.922	-1.685.619	15	114
Amortizacija	-1.181.948	-1.089.838	9	108
Stroški dela	-7.688.723	-6.855.174	62	112
Drugi odhodki	-241.152	-170.282	2	142
SKUPAJ ODHODKI	-12.465.626	-11.158.056	100	112

REZULTAT POSLOVANJA	94.069	544.392	-	17
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Finances

REVENUES (EUR)

	2007	2006	Structure 2007 (%)	Index 2007/2006
Research programmes	3.683.356	3.629.904	29	101
Infrastructure programmes	407.598	418.777	3	97
Research projects	1.196.812	1.129.784	10	106
Overhead financing	1.530.986	1.501.269	12	102
Young researchers	1.745.867	1.278.041	14	137
Domestic market	2.549.295	2.416.579	20	105
Foreign market	550.659	413.784	4	133
Other incomes	895.120	914.310	7	98
TOTAL	12.559.695	11.702.447	100	107

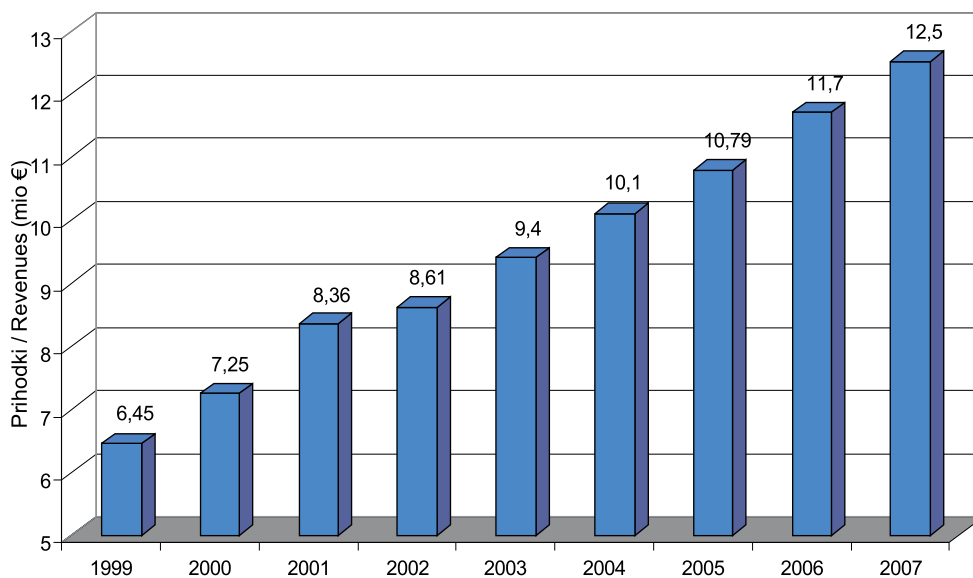
OUTFLOW (EUR)

	2007	2006	Structure 2007 (%)	Index 2007/2006
Costs of material	-1.439.881	-1.357.143	12	106
Costs of services	-1.913.922	-1.685.619	15	114
Depreciation	-1.181.948	-1.089.838	9	108
Labour costs	-7.688.723	-6.855.174	62	112
Other outcomes	-241.152	-170.282	2	142
TOTAL	-12.465.626	-11.158.056	100	112

FINAL RESULT	94.069	544.392	-	17
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Prihodki Kemijskega inštituta

Revenues of the National Institute of Chemistry



SLIKA

Prihodki Kemijskega inštituta v mio EUR.

FIGURE

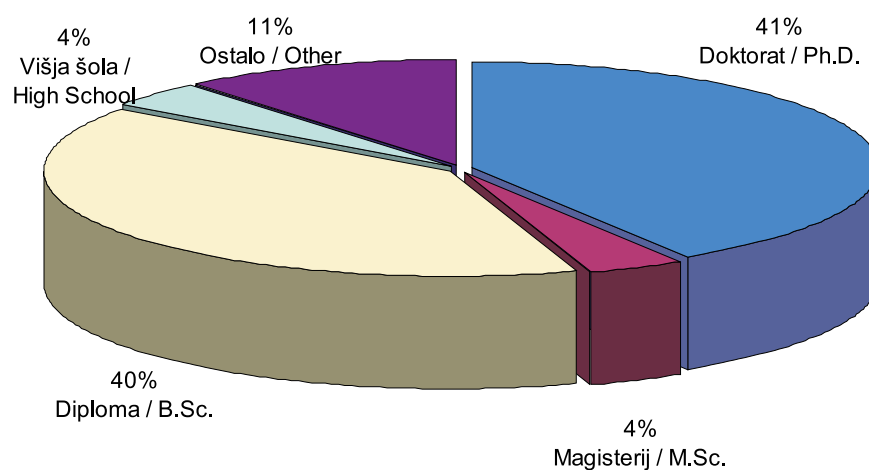
Revenues of the National Institute of Chemistry in million euros.

Zaposleni

Personnel

Na dan 31. 12. 2007 je bilo na Kemijskem inštitutu 256 zaposlenih, od tega 104 doktorji znanosti, 9 magistrov, 102 z visoko izobrazbo, 10 z višjo izobrazbo, 22 s srednjo in 9 z nižjo izobrazbo. Število zaposlenih se je glede na predhodno leto povečalo za 6 %, predvsem na račun uspešnih prijav na razpis za mlade raziskovalce.

On December 31st 2007, we have recorded 256 employees with the following degree of education: Ph.D. (104), Master degree (9), Bachelor degree (102), Associate degree (10), secondary school (22) and less than secondary school (9). Compared to the previous year the number of employees rose by 6 %, mainly due to a number of successful applications for the "Young Researcher" tender.



SLIKA
Izobrazbena struktura zaposlenih na Kemijskem inštitutu v letu 2007.

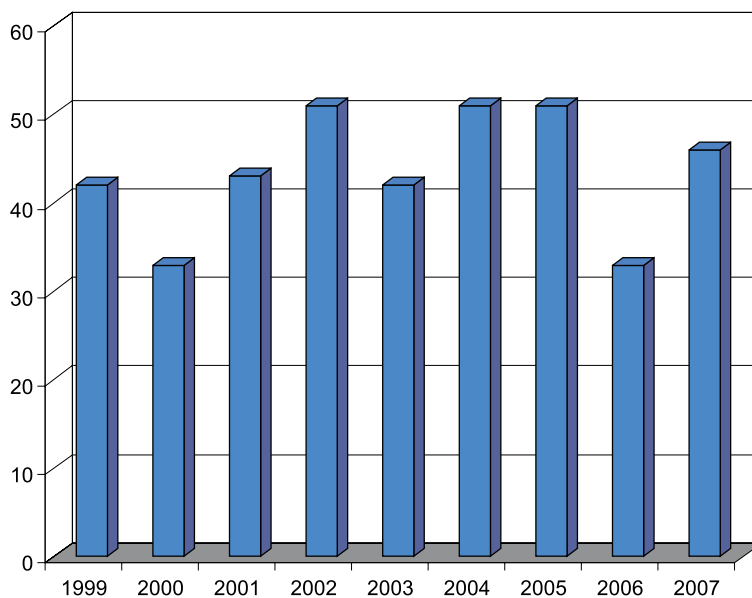
FIGURE
Employees level of education at the National Institute of Chemistry in 2007.

Doktorati, magisteriji in diplome v letu 2007

Doctoral, Master's and Graduate Theses in Year 2007

DOKTORATI / DOCTORAL THESES

- Luka Zevnik, 11.1.2007
- Borštnik Urban, 21.5.2007
- Japelj Boštjan, 7.6.2007
- Vasko Jovanovski, 13.6.2007
- Butinar Lorena, 15.10.2007
- Mohorčič Martina, 26.10.2007
- Križman Mitja, 21.11.2007
- Vince Jelica, 23.11.2007
- Strmčnik Dušan, 19.12.2007
- Bren Urban, 21.12.2007



SLIKA
Doktorati, magisteriji in diplome v letih
1999 / 2007.

FIGURE
Ph.D., M.Sc., and B.Sc. theses in years
1999 / 2007.

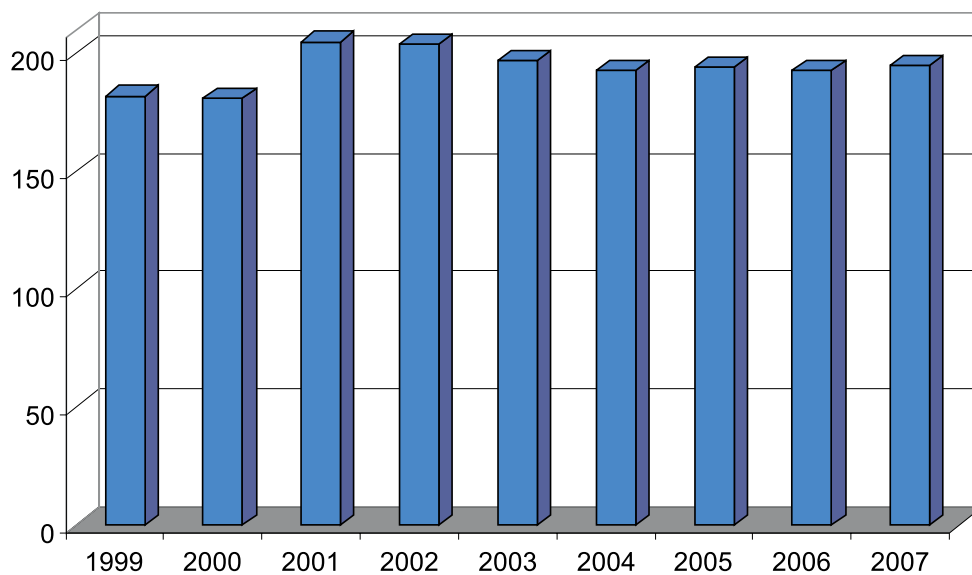
**ŠTEVILO DIPLOM, MAGISTERIJEV, DOKTORATOV, MENTORSTEV IN KOMENTORSTEV S
STRANI ZAPOSLENIH NA KEMIJSKEM INŠTITUTU**

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

- 1 diploma / Undergraduate Thesis
- 10 doktoratov / Doctoral Theses
- 7 mentorstev pri diplomah / Mentorships of Undergraduate Theses
- 2 mentorstvi pri magisterijih / Mentorships of Master's Theses
- 11 mentorstev pri doktoratih / Mentorships of Doctoral Theses
- 21 komentorstev pri diplomah / Comentorships of Undergraduate Theses
- 1 komentorstvo pri magisterijih / Comentorship of Master's Theses
- 5 komentorstev pri doktoratih / Comentorships of Doctoral Theses

Objave v letu 2007

Published Works in Year 2007



SLIKA
Objavljena dela (članki, knjige, poglavja, patenti) v letih 1999 / 2007.

FIGURE
Published works (papers, books, chapters, patents) in years 1999 / 2007.

Bibliografija inštituta v letu 2007
ANALITIČNI PODATKI (tipologija COBISS /
laboratoriji)

Institute bibliography for 2007
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	47	38	15	8	17	8	11	2	12	28	12	26	8	3	7	242	16	226
Prispevki na konferencah / Conference contributions	48	36	33	14	23	11	37	0	19	17	43	22	7	3	10	323	20	303
Patenti / Patents	0	1	0	0	1	0	3	1	0	1	2	3	0	0	0	12	1	11
Predavanja / Lectures	17	3	3	0	6	2	3	0	2	2	4	7	1	0	4	54	1	53
Dokumenti / Documents	2	4	0	5	14	1	4	0	1	6	0	0	1	8	0	46	0	46
Doktorati, magisteriji, diplome / PhD, MSc, BSc	3	6	2	1	4	5	2	0	2	4	3	9	3	2	0	46	0	46
SKUPAJ / ALL UNITS	117	88	53	28	65	27	60	3	36	58	64	67	20	16	21	723	38	685

Mednarodno sodelovanje

International Cooperation

MULTILATERALNO SODELOVANJE / MULTILATERAL COOPERATION

6. Okvirni program EU / EU 6th Framework Program	14
Leonardo da Vinci	1
TEMPUS	1
ERA-NET	1
COST	3
PROTEUS	2
Skupno / Total	22

BILATERALNO SODELOVANJE / BILATERAL COOPERATION

Argentina / Argentine	1
Ciper / Cyprus	1
Češka / Czech Republic	2
Hrvaška / Croatia	5
Indija / India	2
Italija / Italy	1
Izrael / Israel	1
Japonska / Japan	1
Madžarska / Hungary	2
Makedonija / Macedonia	3
Norveška / Norway	1
Romunija / Romania	1
Srbija / Serbia	2
Turčija / Turkey	1
Velika Britanija / Great Britain	2
ZDA / USA	6
Skupno / Total	32

Nagrade in priznanja podeljena sodelavcem inštituta v letu 2007

Awards and Recognition of Collaborators of the National Institute of Chemistry in 2007

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

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



Slavnostni govornik na dogodku je bil premier Janez Janša

The Honorary Speaker was the Prime Minister of Slovenia Janez Janša



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

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



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

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



Preglovo nagrado Kemijskega inštituta za izjemno doktorsko delo na področju kemije in sorodnih ved je prejel dr. Vasko Jovanovski; 13. 12. 2007.

The Pregl Award of the National Institute of Chemistry for outstanding doctoral work in the field of chemistry and related sciences was awarded to Dr. Vasko Jovanovski; December 13, 2007.

Naziv častni član Kemijskega inštituta je bil podeljen:

The Naming of an Honorary Member of the National Institute of Chemistry was given to:



- **prof. Josephu Wangu** za dolgoletno plodno sodelovanje z raziskovalci Kemijskega inštituta, za njegov neprecenljiv prispevek k ugledu inštituta in njegove izjemne dosežke na področju elektrokemije in razvoja kemijskih senzorjev. (Ljubljana, 15. 6. 2007)

- **Professor Joseph Wang**, for his many years of fertile research collaboration with the researchers of the National Institute of Chemistry, for his invaluable contribution to the reputation of the Institute, and his exceptional achievements in the field of electrochemistry and the development of chemical sensors. (Ljubljana, June 15, 2007)



- **prof. Milanu Randiću**, za njegov neprecenljiv prispevek k promociji Kemijskega inštituta in slovenske znanosti na področju računalniške kemije. (Ljubljana, 27. 9. 2007)
- **Professor Milan Randić**, for his invaluable contribution to the promotion of the National Institute of Chemistry and Slovenian science in the field of computational chemistry. (Ljubljana, September 27, 2007)

ZOISOVE NAGRADE IN PRIZNANJA 2007,
22. 11. 2007

ZOIS PRIZE AND RECOGNITION 2007,
November 22, 2007



Docent dr. Janko Jamnik je prejel Zoisovo priznanje za pomembne dosežke na področju znanosti o materialih.

Dr. Janko Jamnik, Assist. Prof. received the Zois Recognition for important achievements in the area of materials science.

Tekmovanje iGEM (international Genetically Engineered Machines), na univerzi Massachusetts Institute of Technology (MIT), Cambridge, ZDA; 3. – 4. 11. 2007

iGEM Competition (international Genetically Engineered Machines), at the Massachusetts Institute of Technology (MIT), Cambridge, USA; November 3 – 4, 2007



Slovenska ekipa študentov je na tekmovanju raziskovalnih projektov na področju sintezne biologije z novim pristopom zdravljenja okužbe z virusom HIV osvojila **prvo mesto na področju zdravja in medicine**, kar je ponovitev izjemnega uspeha iz leta 2006.

Zasnova in raziskovalno delo projekta sta pod mentorskim vodstvom potekala na Kemijskem inštitutu. Mentorji so prejeli **nagrado Prometej znanosti za znanstveno komuniciranje**, ki jo podeljuje Slovenska znanstvena fundacija ter **Sokratovo odličje za visokošolsko didaktiko**.

Več na strani 161

Team of Slovenian undergraduate students together with their mentors from the National Institute of Chemistry Slovenia.

The team **won the first prize for the project in the field of Health and Medicine**, repeating the success at this competition from the previous year. Young Slovenian synthetic biologists devised a mutation-independent defence against HIV.

The mentors obtained **the Prometheus Scientific Award for scientific communication** granted by Slovenian Scientific Foundation, and **Socrates Award for high education didactics**.

More: page 161

37. Krkine nagrade 2007; Novo mesto, 19. 10. 2007

- **dr. Mateja Novak Štagoj** je prejela nagrado za posebne dosežke na področju raziskovalnega dela. Nagrado je prejela za doktorsko delo z naslovom "Heterologna ekspresija iz promotora GAL1 v načrtovanih mutantah kvasovke *Saccharomyces cerevisiae*", somentor: prof. dr. Radovan Komel.
- **Monika Ciglič** je prejela nagrado za diplomsko delo z naslovom: »Vpliv sprememb MYD88 na signalizacijo Tollu-podobnih receptorjev«; mentor: prof. dr. Roman Jerala.

Prešernove nagrade študentom Fakultete za kemijo in kemijsko tehnologijo, Univerza v Ljubljani; december 2007

- **Alen Kljajić**, za diplomsko delo: "Sinteza antimonovih mezoporoznih silikatov"; somentor: prof. dr. Venčeslav Kaučič.
- **Tilen Nastran**, za diplomsko delo: "Stacionarni model nizkotemperaturne gorivne celice s protonsko izmenjalno membrano"; mentor: akademik prof. dr. Janez Levec; delovni mentor: dr. Stanko Hočevar.

37. Krka Prize 2007; Novo Mesto, October 19, 2007

- **Dr. Mateja Novak Štagoj** received the prize for special achievements in research. She received the award for her doctoral work entitled "Heterologous expression in designed mutant strains of yeast *Saccharomyces cerevisiae* using the GAL1 promoter", co-mentor: Professor Radovan Komel.
- **Monika Ciglič** received the award for her undergraduate degree work entitled "The effect of modification of protein MYD88 on Toll-like receptor signaling"; mentor: Professor Roman Jerala.

The Prešeren Prize to students from the Faculty of Chemistry and Chemical Technology, University of Ljubljana; December 2007

- **Alen Kljajić**, for his undergraduate research degree work entitled: "Synthesis of antimony mesoporous silicates"; co-mentor: Professor Venčeslav Kaučič.
- **Tilen Nastran**, for his undergraduate research degree work entitled: "Stationary model of low-temperature PEMFC"; mentor: Professor and Member of the Academy of Sciences Janez Levec, PhD; working mentor: Dr. Stanko Hočevar.

Zaposleni v splošnem sektorju

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do / until 31.7.2007)
Robert Vidmar (vodja / head,
od / since 1.8.2007)
Toni Ambrož
Gregor Babnik

Marjan Smole
Pavle Vrhovec

RAČUNOVODSTVO, PLAN IN ANALIZE / ACCOUNTING, PLANNING AND ANALYSES

Barbara Dorić
Zlatka Skok
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Splošni sektor
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Alen Kljajić
Peter Miklavc
Špela Miklavič
David Perko
Andrej Tehovnik

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

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Nejc Carl
Martina Glušič
Janez Konc
Borut Tone Oblak
Andrej Perdih
Gordana Pirc
Mihael Simčič
Tjaša Urbič
Jernej Zidar

TEHNIČNO OSEBJE / TECHNICAL STAFF

Tatjana Karba
Silva Zagorc



PODROČJA DEJAVNOSTI

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 P1-0010 (F. Avbelj)

Folding in dinamika biomolekularnih sistemov

- Raziskave strukture in dinamike biomolekularnih sistemov (proteinov, ligandov, mem-

RESEARCH ACTIVITIES

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 and 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 P1-0010 (F. Avbelj)

Protein folding and dynamics of biomolecular systems

- bran 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)
 - 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 P1-0002: (D. Janežič)

Računalniško modeliranje strukture in dinamike molekul

Raziskovalna projekta:

- **J1-6331:** (D. Janežič)

Razvoj računalniških algoritmov za simulacije makromolekularnih sistemov

- **J1-9804:** (F. Merzel)

Računalniške simulacije in analiza kolektivnih gibanj biomolekul

Razvoj in uporaba metod za molekularno modeliranje:

- Simplektične metode za simulacijo molekulske dinamike makromolekul
- Kombinacije metod simulacije molekulske dinamike, analize po normalnih načinih ni-

- 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 vibrational 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 P1-0002: (D. Janežič)

Computer simulation of molecular structure and dynamics

Research projects:

- **J1-6331:** (D. Janežič)

Computer Algorithms Development for Macromolecular Simulation

- **J1-9804:** (F. Merzel)

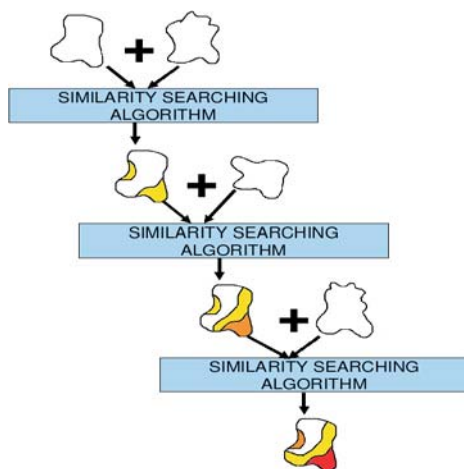
Computer simulations and analysis of collective motions of biomolecules

hanja in kvaziharmonske analize proteinov v raztopinah za študij hidracije 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 računalniške gruče

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



SLIKA 1:

Leva slika: Shematska predstavitev novega algoritma za napovedovanje proteinskih vezavnih mest. Struktura evolucijsko povezanih proteinov zaporedoma primerjamo z izbranim proteinom. Ugotovljene podobnosti potem preslikamo na površino izbranega proteina. Desna slika: Najboljša konformacija nevezanega liganda (rdeča) sidrana na tarčni protein (zelen) in znana kristalna struktura proteinskega kompleksa (veriga A, modra; veriga B, skriljasta). Napovedano vezavno mesto sidranega liganda je škrlatno.

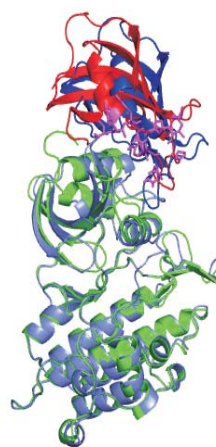


FIGURE 1:

Left figure: Protein-protein binding sites prediction procedure. Structures of related proteins are sequentially compared with the query protein. The found similarities are mapped on the surface of the query protein. Right figure: The best conformation of unbound ligand (red) docked to target protein (green) and the known crystal structure of the protein complex (chain A, blue; chain B, slate). The predicted binding site residues of docked ligand in magenta.

BIBLIOGRAFIJA

- 39 izvirnih znanstvenih člankov
- 2 strokovna članka
- 1 poljudni članek
- 1 samostojni znanstveni sestavek v monografiji
- 1 intervju
- 1 drugi članki ali sestavki
- 1 znanstvena monografija
- 1 drugo učno gradivo
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanja)
- 1 objavljeni znanstveni prispevek na konferenci
- 45 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 9 predavanj na tujih univerzah
- 4 prispevki na konferencah brez natisa
- 4 vabljeni predavanja na konferencah brez natisa
- 2 končni poročili o rezultatih raziskav
- 3 doktorati
- 3 uredništva revij

GLAVNI DOSEŽKI V LETU 2007

- Študirali smo kemijsko reakcijo med aflatoksinom (najbolj karcinogen snov) in DNA. Uporabili smo post Hartree-Fockove in DFT kvantno kemijske metode z različnimi modeli solvatacije. Izračunana reaktivnost je v odličnem soglasju z eksperimentalno konstanto hitrosti reakcije. Pokazali smo, da je furofuranski del molekule odgovoren za visoko reaktivnost in s tem povezano karcinogenost mikotoksina.
- Z uporabo Thielejevih kumulantov smo razvili novo metodologijo za razcep proste energije vezave. Metoda predstavlja ključno povezavo med strukturo in biološko aktivnostjo molekul. Pomembna je za racionalno načrtovanje učinkovin in bo zagotovo mesto našla v farmacevtski industriji. Z izračuni proste energije v kombinaciji s simulacijo molekulske dinamike smo študirali DNA polimerazo. Jakost vodikove vezi med ligandom

- Development and use of the RISM formalism
- Development of new and effective network topologies for connecting personal computers into computational clusters

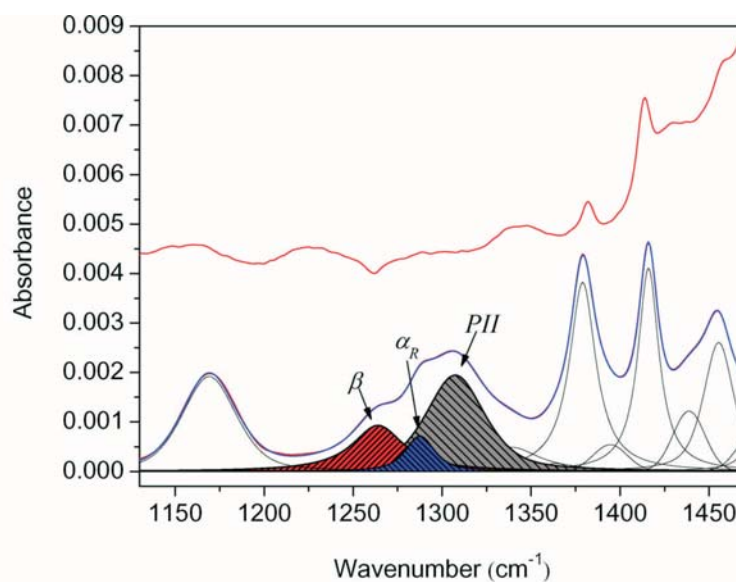
BIBLIOGRAPHY

- 39 Original Scientific Articles
- 2 Professional Articles
- 1 Popular Article
- 1 Independent Scientific Component Part in a Monograph
- 1 Interview
- 1 Other Articles or Component Parts
- 1 Scientific Monograph
- 1 Other Educational Material
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 1 Published Scientific Conference Contribution
- 45 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 9 Invited Lectures at Foreign Universities
- 4 Unpublished Conference Contributions
- 4 Unpublished Invited Conference Lectures
- 2 Final Research Reports
- 3 Doctoral Dissertations
- 3 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2007

- We studied chemical reaction between the most carcinogenic substance aflatoxin and DNA using advanced quantum chemical methods in conjunction with various solvation models. The calculated reactivity is in a very good agreement with the experimental value. Our study gave evidence that furofuran moiety is responsible for reactivity and therefore associated carcinogenicity of the mycotoxin.
- We developed a novel method for decomposition of free energy of binding based on Thiele cumulants. The method provides key link between structure and binding free energies.

- in encimom je odgovorna za visoko zanesljivost podvajanja DNA. Pokazali smo na pomen preorganizirane elektrostatike.
- Dinamiko vodikovo vezanih sistemov smo študirali z Car-Parrinello metodo. Asimetrični OH stretching smo kvantizirali, ostale prostostne stopnje pa obravnavali klasično. Razvito metodologijo smo uporabili za Mannichovo bazo v trdnem in raztopini ter za študij vodikove vezi v hidrogen sulfatu. Delali smo na nadaljnem razvoju numeričnega reševanja vibracijske Schroedingerjeve enačbe. Kritično smo primerjali različne ortogonalizacijske procedure za vibracijske bazne sete. Študirali smo efekte reduciranih mas v internih koordinatah. Z uporabo mešane kvantno-klasične dinamike smo obravnavali katalitično stopnjo lipoksigenaze. Reproducirali smo visok H/D kinetični izotopski efekt 81.
 - Naše študije kemijsko denaturiranega proteina ubiquitin in dipeptidov so pokazale, da aminokislinski ostanki v denaturiranih proteinih in dipeptidih zavzamejo predvsem P_{II}
 - The developed methodology is relevant for drug design and may be of interest for pharmaceutical industry. Using free energy calculations in the framework of molecular dynamics simulation we established the importance of a hydrogen bond strength in the complex between DNA polymerase and a ligand. The study provides evidence about role of pre-organized electrostatics in the process of DNA fidelity.
 - Dynamics of hydrogen bonds was studied by Car-Parrinello simulation. The OH asymmetric stretching was quantized, while the other degrees of freedom were considered to be classical. We applied the methodology to hydrogen sulfate in solid state and Mannich base in the solid state and solution. We further developed methodology for numerical solving of vibrational Schroedinger equation that include critical comparison of various orthogonalization procedures for vibrational basis sets and advanced treatment of reduced masses. Using mixed quantum-classi-



SLIKA 2:

Dekompozicija amidnega III območja alanin dipeptida v H_2O (200 mM). Spekter alanin dipeptida v D_2O je v rdeči barvi.

FIGURE 2:

Decomposition of the Amide III region of alanine dipeptide in H_2O (200 mM). The red spectrum represents the same dipeptide in D_2O .

in β konformaciji. Pokazali smo tudi, da se v denaturiranih proteinih lahko tvorijo zametki β -trakov, kar lahko povzroča nastanek fibrilov. V nasprotju s temi eksperimentalnimi rezultati pa teoretske metode, kot so Amber, CHARMM, Discover in GROMOS, napovedujejo večji ali celo dominanten delež α_R konformacije v nestrukturiranih peptidih in proteinih. Odkrili smo, da potenciali Lennard-Jones, ki se uporabljajo v teh programih, nepravilno opišejo nevezne interakcije v peptidih. Na osnovi potencialov srednje sile smo razvili nov Exp-6 potencial za nevezne interakcije v proteinih, ki je zelo uspešen pri napovedovanju struktur majhnih peptidov.

- Izolirali in proučevali smo relevantni encim za študij vezave novih ligandov za razvoj novih antibiotikov; izpopolnili smo NMR meritve, ki temeljijo na opazovanju signalov liganda in natančno določili vezavno afiniteto novih ligandov.
- Z uporabo vibracijske spektroskopije smo raziskovali konformacijske preference 13 blokiranih dipeptidov. Pokazali smo, da frekvenca amidnega I traku in razmerje integralnih intenzitet njegovih komponent korelirata z $^3J(H_N, H_\alpha)$ sklopitvenimi konstantami. Opisana spektralna parametra lahko uporabimo za določevanje torzijskega kota ϕ . Prisotnost populacij P_{II} , β , and α_R konformer smo določili z analizo ramanskih skeletnih nihanj in infrardečega amidnega III traku. Alanin dipeptide se nahaja večinoma v P_{II} konformaciji. V dipeptidu valina naraste delež β konformacije. Populacija α_R konformacije je v obeh dipeptidih majhna. Predstavljeni rezultati potrjujejo model elektrostatskega senčenja konformacijskih preferenc aminokislinskih ostankov.

V okviru dela na raziskovalnem programu P1-0002 smo v letu 2007 objavili 20 originalnih znanstvenih člankov, vse v SCI revijah, od katerih jih je 14 v SCI revijah iz prvega kvartila. Objavili smo tudi znanstveno monografijo. Nekateri glavni dosežki so naslednji:

cal dynamics we studied catalytic step of lipoxygenase. The unusual H/D isotope effect of 81 was successfully reproduced

- Our experimental studies of chemically denatured ubiquitin have shown that residues in unstructured proteins adopt mainly the P_{II} in β conformations. Nascent native-like β -strands in denatured proteins may even nucleate fibril formation. In contrast, theoretical studies using: Amber, CHARMM, Discover, and GROMOS, predict that population of the α_R conformation in unstructured proteins and peptides is large. We have shown that the Lennard-Jones potentials, usually used in theoretical studies, cannot adequately describe non-bonded interactions in peptides. We developed a new Exp-6 potential for proteins, which is successful in predicting structure of small peptides.
- We have investigated binding of new ligands to a relevant enzyme, which is an appropriate target for the development of new antibiotics. NMR measurements based on observation of ligand resonances have been improved for precise determination of ligand binding affinities.
- We studied the conformational preferences of 13 dipeptides using infrared and Raman spectroscopy. We showed that the frequencies of Amide I band and the A_{12} ratio of Amide I components of dipeptides correlate with the $^3J(H_N, H_\alpha)$ NMR coupling constants. These two IR vibrational parameters are thus, analogous to $^3J(H_N, H_\alpha)$, indicators for the preference for the dihedral angle Φ . We also showed that the intensities of the components of the Amide III bands in IR spectra and the intensities of the skeletal vibrations in Raman spectra are indicators of populations of the P_{II} , β , and α_R conformations. The results show that alanine dipeptide adopts predominantly the P_{II} conformation. The population of the β conformation increases in valine dipeptide. The populations of the α_R conformation are generally small. These data

- Študirali smo povezave med teorijo matrik in teorijo grafov ter uporabo teorije grafov v kemijski in bio informatiki. Objavili smo znanstveno monografijo z naslovom *Graph Theoretical Matrices in Chemistry*, prvo znanstveno knjigo na področju kemijske teorije grafov, to je veje matematične kemije, ki direktno uporablja matematično teorijo grafov.
 - Z uporabo teorije proteinskih grafov smo razvili nov pristop za iskanje funkcijsko pomembnih predelov proteinov, ki je še posebej primeren za iskanje vezavnih mest, s katerimi se proteini povezujejo z drugimi proteini. Novo razviti pristop temelji na primerjavi struktur proteinov, s pomočjo katere je mogoče poiskati v evoluciji strukturno ohranjene površinske aminokislina. Naš pristop napovedovanja vezavnih mest na proteinih, ki napoveduje proteinska vezavna mesta bolj hitro in bolj nepristransko kot druge znane metode, bo pripomogel k iskanju in karakterizaciji ključnih področij na proteinih, na katerih potekajo interakcije protein-protein in bi lahko bila primerna kot mesta za razvoj novih zdravilnih učinkovin.
 - Končali smo z razvojem novega empiričnega polja sil za simulacijo molekulske dinamike fleksibilne kristalne rešetke alumofosfata $\text{AlPO}_4\text{-34}$. Z razvitim poljem sil smo izvedli simulacijo molekulske dinamike alumofosfata in izračunali Debye-Wallerjeve faktorje ter IR spekter alumofosfata. Pokazali smo, da molekule templata prispevajo k večji stabilnosti kristalne rešetke.
 - Razvili smo metodo in programski paket "NMscatt" za računanje spektrov neelastičnega nevtronskega sipanja biomolekul na podlagi klasičnih simulacij. Metoda je služila kot osnovno orodje pri študiju razpiranja baznih parov pri molekuli DNK. Pokazali smo, da lahko z uporabljenim atomskim modelom DNK s potencialnim poljem sil Charmm zelo dobro reproduciramo izmerjeno disperzijsko zvezo za valovanje vzdolž vijačne osi DNK molekule. Ugotovili smo, da vibracijski načini are in accord with the electrostatic screening model of conformational preferences.
- As part of the work under the research program P1-0002 we published 20 original scientific articles, which all appear in SCI journals and 14 of which are in the first quartile of SCI journals. We also published a scientific book. Some of the major achievements are the following:
- We have studied the relationship between matrix theory and graph theory, as well as the use of graph theory in chemical- and bio-informatics. We published the scientific monography *Graph Theoretical Matrices in Chemistry*, the first scientific book in the subject of graph theory in Chemistry, an area of mathematical chemistry directly using mathematical graph theory.
 - By using the theory of protein graphs, we have developed a new approach to finding the protein areas that are functionally important. The approach is ideally suited to finding protein-protein binding sites. The newly-developed method is based on comparing the protein structures to determine the amino acids on the protein surface that have been structurally conserved through evolution. Our approach to predicting protein binding sites is faster and less biased than other known approaches. These advantages will enable to find and characterize the key protein sites that are present in protein-protein interactions and which may be targeted for new drugs.
 - We developed a new empirical force field for an all-atom MD simulation of a flexible $\text{AlPO}_4\text{-34}$ triclinic framework. Using the force-field we have performed an MD simulation of the aluminophosphate and computed the Debye-Waller's factors and the IR spectrum. We have shown that the templating molecules contribute to a higher stability of the crystalline framework.
 - We have developed program package "NMscatt" for calculating inelastic neutron

podobni "dihanju" DNK molekule (i.e. razmikanje baznih parov) niso lokalizirani na posamezne frekvence, temveč da obstaja zvezno območje (pas) vibracijskih stanj, 50-300 cm⁻¹ s takšnim značajem. S pomočjo programskega paketa "NMscatt" smo s sodelavci iz Univerze Heidelberg študirali tudi mrežna nihanja kristaliziranega proteina ribonukleaze. Pokazali smo, da je glavni prispevek k razširitvi Braggovih črt na račun akustičnih fononov.

- V sodelovanju z Max-Planck Institute for Polymer Research, Mainz, Nemčija smo razvili adaptivno simulacijsko shemo (Adaptive Resolution Scheme), ki omogoča spremembo krajevne resolucije med samim potekom simulacije molekulske dinamike. Metoda omogoča, da poenostavimo fizikalni opis sistema do največje dopustne stopnje. Pri tem pri obravnavi molekularnega sistema ohranimo vse podrobnosti opisa sistema v tistih območjih, kjer je to potrebno. Metodo smo razširili z vključitvijo sil dolgega dosega, t.j., elektrostatskih sil. Ta korak je iz metodološkega vidika izredno pomemben, ker omogoča obravnavo polarnih topil, npr. tekoče vode kot najpomembnejšega topila v naravi. Ker se porabi večina (tudi do 90%) računalniškega časa pri simulaciji molekulske dinamike makromolekule v eksplicitnem topilu za izračun dinamike topila in ne makromolekule, smo razvili pristop, kjer topilo obravnavamo na atomski skali le v neposredni okolici makromolekule (nekaj solvacijskih lupin), medtem ko topilo dlje stran opišemo na bolj grobozrnati stopnji. S tem znatno povečamo učinkovitost simulacije. Novo metodo smo uporabili za simulacijo molekulske dinamike generične makromolekule v topilu in na sistemu molekul vode. Pokazali smo tudi, da opisani pristop vodi do koncepta geometrijsko inducirane faznega prehoda in razširitve ekvipartijskega izreka na necele prostostne stopnje.
- Dr. Dušanka Janežič je Associate Editor revije

and X-ray scattering from the classical simulations. The method was used as a main tool for the investigation of the breathing like modes of the DNA molecule. We have shown that the calculated dispersion relation at the low frequency from the fully atomistic model of DNA using the CHARMM force field agrees excellently with experimental data. We have found a continuous band of modes with strong base-pair opening up to 300 cm⁻¹. Using "NMscatt" we have provided all-atom lattice dynamical calculations for a crystalline protein, ribonuclease A. In the Bragg peak vicinity, inelastic scattering of X-rays by phonons is found to originate from acoustic mode scattering.

- In collaboration with the Max Planck Institute for Polymer Research, Mainz, Germany we have developed a new adaptive simulation scheme (AdResS), which allows for changing the spatial resolution during the course of a molecular dynamics (MD) simulation. In this way one can simplify the physical description of the system under study to the largest extent possible while retaining all the details of the system where this is necessary. The approach was extended to also treat the long-range forces, i.e., electrostatic interactions. This methodological step is of a significant importance since it allows us to simulate also polar solvents, e.g., liquid water as the most important solvent in nature. It is well known that the most (up to 90%) of CPU time is required in a simulation of a macromolecule solvated in an explicit solvent to compute dynamics of the solvent (and not the macromolecule). To circumvent this problem we have developed an approach, where the solvent is treated explicitly only in the very vicinity (a few solvation shells) of the macromolecule while farther away a more coarse-grained description is used for the solvent. Using this approach the efficiency of a simulation is greatly enhanced. The new method was used for an MD simulation of a generic macromolecule in a solvent and for a system

Journal of Chemical Information and Modeling (JCIM), An American Chemical Society Publications. V letu 2007 je poleg rednega uredniškega dela uredila še posebno številko JCIM-a posvečeno akademiku profesorju Nenadu Trinjastiću (Vol. 47, No. 3, 2007).

- Dr. Dušanka Janežič je postala članica Editorial Board-a: Advances in Chemoinformatics and Computational Methods (ACCM), Book Series, IGI Global, MIT Press.
- Dr. Milan Hodošček je soavtor in razvijalec najbolj uporabljanega računalniškega programa za molekularno modeliranje - CHARMM (Chemistry at HARvard Molecular Mechanics).

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Lek d.d. (doc. dr. Simona Golič Grdadolnik)
- Krka d.d., Novo mesto (doc. dr. Jože Grdadolnik)

Pri raziskavah, ki jih izvajamo v okviru našega raziskovalnega dela v Centru za molekularno modeliranje na Kemijskem inštitutu, v sodelovanju s firmo Lek, d.d., Raziskave učinkovin, delamo na projektih raziskav za obdelavo NMR spektrov in molekularnega modeliranja kot pomoč pri interpretaciji NMR spektrov (dr. Dušanka Janežič). Sodelujemo tudi z z Inštitutom Jožef Stefan, Medicinsko fakulteto Univerze v Ljubljani, Fakulteto za matematiko in fiziko Univerze v Ljubljani, Biotehniško fakulteto Univerze v Ljubljani, Filozofsko fakulteto Univerze v Ljubljani, Fakulteto za računalništvo in informatiko Univerze v Ljubljani.

MEDNARODNO SODELOVANJE

- Slovensko-ciprski bilateralni projekt: Odkrivanje fenomena zvitja proteinov preko konformacijske analize majhnih linearnih peptidov (nosilca S. Golič Grdadolnik in T. Mavromoustakos)
- Slovensko-hrvaška bilaterala 2007-2008 (doc. dr. Jože Grdadolnik)

of liquid water. We also demonstrated that the described approach leads to a concept of geometry induced phase transition and a generalization of the equipartition theorem to fractional degrees of freedom.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Lek d.d., Slovenia (Dr. Simona Golič Grdadolnik)
- Krka d.d., Novo mesto, Slovenia (Dr. Jože Grdadolnik)

In collaboration with Lek d.d. Slovenia, a Sandoz company, Drug Discovery we develop novel chemical entities (NCE's) in the antiinfective and cardiovascular therapeutic areas and we also collaborate on research projects for processing NMR spectra using molecular modeling approaches (Dr. Dušanka Janežič). We collaborate also with Institute Jožef Stefan, Slovenia, the Faculty of Medicine, the Faculty of Mathematics and Physics, the Biotechnical faculty, the Faculty of Arts, the Faculty of Computer and Information Science (all members of University of Ljubljana, Slovenia).

INTERNATIONAL COLLABORATION

- Slovenian-Cypriot bilateral project: Approaching the Protein Folding Through Conformational Analysis of Small Linear Peptides (Principal investigators: Dr. Simona Golič Grdadolnik and Dr. T. Mavromoustakos)
- Bilateral cooperation Slovenia-Croatia 2007-2008 (Dr. Jože Grdadolnik)

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

Kemijski inštitut, Center za molekularno modeliranje (dr. Dušanka Janežič, dr. Milan Hodošček) in RIKEN Yokohama Institute, High Performance Molecular Simulation Team, Japonska sta podpisala tri letni sporazum o znanstveno raziskovalnem sodelovanju (Collaborative Research Agreement) na področju razvoja namenske strojne in programske opreme za izvajanje simulacij molekulske dinamike bioloških makromolekul. Tovrstno sodelovanje potrjuje, da smo med vodilnimi svetovnimi razvijalci vzporednih računalniških gruč za izvajanje vzporednih simulacij molekulske dinamike velikih sistemov, ki jih uspešno uvajamo v Sloveniji in tako slovenskim raziskovalcem omogočamo dostopnost do vrhunske strojne in programske opreme. Sodelujemo na financiranih bilateralnih projektih, katerih odgovorna nosilka je dr. Dušanka Janežič, z raziskovalci iz naslednjih držav:

- z ZDA: dr. Bernard R. Brooks, National Institutes of Health, Bethesda, MD;
- s Hrvaško:
 - dr. Sonja Nikolić, Institute Rudjer Bosković, Zagreb;
 - dr. Sanja Tomić, Institute Rudjer Bosković, 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, Budimpešta, Madžarska (medakademijski projekt);
- s Francijo: Proteus projekt, prof. dr. Mark Johnson, Institute Laue Langevin, Grenoble (odgovorni nosilec dr. Franci Merzel).

POMEMBNI INŠTRUMENTI IN OPREMA

- NMR spektrometri v okviru Slovenskega NMR centra
- FTIR spektrometer z NIR Ramanskim spektrometrom Perkin Elmer System 2000

puter clusters to be used for molecular dynamics simulations of large systems, which we successfully introduced to Slovenia.

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

- USA: Dr. Bernard R. Brooks, National Institutes of Health, Bethesda, MD
- Croatia: Dr. Sonja Nikolić, Institute Rudjer Bosković, Zagreb
- Croatia: Dr. Sanja Tomić, Institute Rudjer Bosković, Zagreb
- Turkey: Dr. Gamze Tanoglu, Izmir Institute of Technology, Izmir
- Romania: Dr. Mircea Diudea, University of Cluj, Cluj
- Hungary: Dr. Istvan Lukovits, Chemical Research Center, Hungarian Academy of Sciences, Budapest
- France: Proteus project, Prof. Dr. Mark Johnson, Institute Laue Langevin, Grenoble (Dr. Franci Merzel).

MAJOR EQUIPMENT

- FTIR spectrometer Perkin Elmer system 2000 with NIR Raman
- FTIR Bruker 66 S
- Glove-box Braun
- NMR spectrometers at Slovenian NMR Center
- We have built the CROW-11 parallel computer cluster from 42 nodes. Each node contains 8 processing cores for a total of 336 processing cores with a speed of 1.9 GHz.
- For greatly speeding up MD simulations, we have used IBM's Cell processor, which is, in its cheapest form, included in the Sony Playstation 3

EDUCATION AND IMPORTANT VISITS

- Dr. Matej Praprotnik has successfully completed his postdoctoral specialization at the Max-Planck Institute for Polymer Research in Mainz, Germany.

- FTIR spektrometer Bruker 66 S
- Suha komora Braun
- Izgradili smo vzporedni računalniški sistem VRANA-11, ki ga sestavlja 42 računalnikov, od katerih vsak vsebuje 8 računskih enot, kar pomeni skupno 336 procesorskih elementov s hitrostjo 1.9GHz.
- Za razvoj zelo hitrega računanja molekulske dinamike smo uporabili IBM-ov processor "Cell", ki je v najcenejši varianti vgrajen v Sony Playstation 3.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Dr. Simona Golič Grdadolnik in dr. Jože Grdadolnik sta bila habilitirana v naziv docenta na Fakulteti za aplikativno naravoslovje Univerze v Novi Gorici;
 - Dr. Matej Praprotnik je uspešno zaključil doktorsko izpopolnjevanje na Max-Planck Institute for Polymer Research v Mainzu, Nemčija;
 - Mladi raziskovalec Urban Borštnik (mentorica dr. Dušanka Janežič) je pridobil naslov doktorja znanosti na Fakulteti za računalništvo in informatiko Univerze v Ljubljani;
 - Mlademu raziskovalcu Janezu Koncu (mentorica dr. Dušanka Janežič) je bila odobrena doktorska tema na Fakulteto za farmacijo Univerze v Ljubljani, kjer je bil tudi izvoljen v naziv asistenta za področje farmacije;
 - Mlademu raziskovalcu Jerneju Zidarju (mentor dr. Franci Merzel) je bil odobren direktni prehod na doktorski študij na Medicinski fakulteti, smer biomedicina, Univerza v Ljubljani;
 - Dr. Dušanka Janežič je bila članica komisije za zagovor doktorata na University of Cluj, Cluj, Romunija;
 - Dr. Franci Merzel je bil član komisije za zagovor doktorata na University of Technology, Delft, Nizozemska.
- Junior Researcher Urban Borštnik (advisor Dr. Dušanka Janežič) has been promoted as a PhD at the Faculty of Computer and Information Science, University of Ljubljana, Slovenia.
 - Junior Researcher Janez Konc's (advisor Dr. Dušanka Janežič) thesis topic has been accepted by the Faculty of Pharmacy, University of Ljubljana, Slovenia, where he was promoted to the position of assistant for pharmacy.
 - Junior Researcher Jernej Zidar (advisor Dr. Franci Merzel) has been granted a direct transition to the PhD program of Biomedicine at the Faculty of Medicine, University of Ljubljana, Slovenia.
 - Dr. Dušanka Janežič was a member of a PhD promotion committee at the University of Cluj, Cluj, Romania.
 - Dr. Franci Merzel was a member of a PhD promotion committee at the University of Technology Delft, The Netherlands.

L02

Laboratorij za spektroskopijo materialov

Laboratory for Spectroscopy of Materials



VODJA / HEAD
dr. Boris Orel

RAZISKOVALCI / RESEARCHERS

dr. Zorica Crnjak Orel
dr. Marta Klanjšek Gunde
dr. Angela Šurca Vuk
dr. Lidija Slemenik Perše
dr. Vasko Jovanovski
dr. Jelica Vince

MLADI RAZISKOVALCI/ YOUNG RESEARCHERS

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Matjaž Koželj
Podbršček Peter
Maša Žveglič

TEHNIČNO OSEBJE / TECHNICAL STAFF

Helena Spreizer
Petra Jamnik (študentsko delo / student work)

PRIPRAVNIKI / TRAINEES

Tanja Boškovič (praksa / practice)
Alenka Sintič (praksa / practice)



PODROČJA DEJAVNOSTI

V Laboratoriju za spektroskopijo materialov razvijamo različne komponente za energetske sisteme, ki izkoriščajo sončno sevanje, pa tudi nanokompozitne materiale za druge aplikacije:

- spektralno selektivni barvni premazi za sončne zbiralnike in fasade zgradb;
- multifunkcionalne nanokompozitne prevleke za tekstil, tudi z baktericidnimi lastnostmi;
- multifunkcionalne nanokompozitne anti-korozijske prevleke za kovine;
- nanostrukturne plasti z interkalacijskimi lastnostmi;
- protonsko prevodne membrane za gorivne celice;
- trdni elektroliti na osnovi ionskih tekočin za elektrokromna (pametna) optično preklopna okna in za Grätzlove fotoelektrokemijske celice;
- priprava nanodelcev na osnovi Cu- in Zn-oxidov;
- razvoj analiznih in eksperimentalnih pristopov za raziskave strukture materialov, optičnih lastnosti (barva, termična emisivnost) in površinskih lastnosti (plazemske tehnologije);

RESEARCH ACTIVITIES

In Laboratory for Spectroscopy of Materials we develop various components for energy systems that exploit solar radiation and, in addition, nanocomposite materials for other applications:

- spectrally selective coloured paint coatings for solar collectors and façades of buildings;
- multifunctional nanocomposite coatings for textile, also with antibacterial properties;
- multifunctional nanocomposite corrosion protective coatings for metals;
- nanostructured layers with intercalation properties;
- proton conductive membranes for fuel cells;
- solid electrolytes on the basis of ionic liquids for electrochromic (smart) optically switchable windows and for Grätzel photo-electrochemical cells;
- preparation of nanoparticles on the basis of Cu- and Zn-oxides;
- the development of analytical and experimental approaches for the investigation of structure of various materials, optical properties (colour, thermal emissivity) and surface properties (plasma technology);

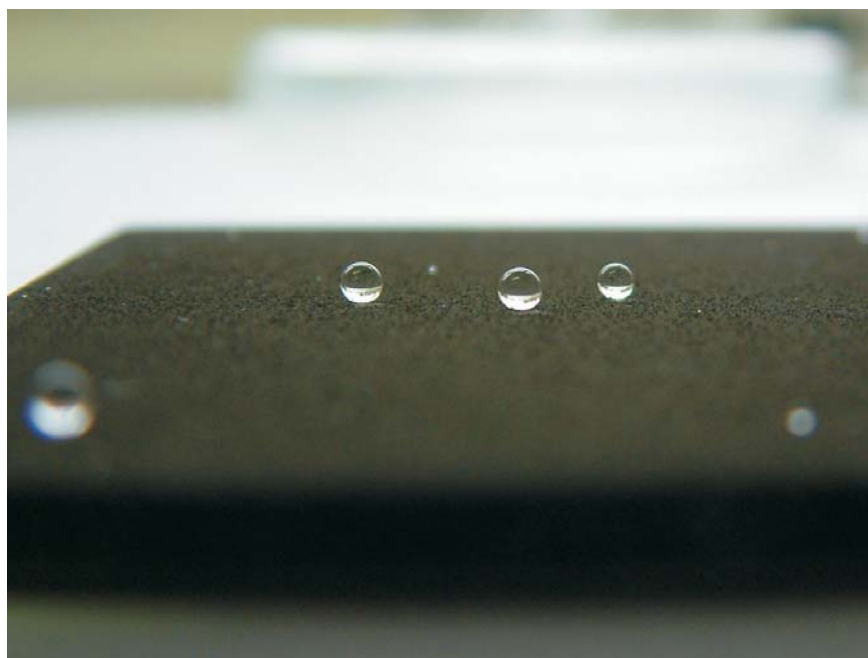
- uporaba reaktivnih in selektivnih plazemskih tehnologij;
 - raziskave materialov, ki so pomembni pri tisku;
 - barve in barvna metrika.
- applications of reactive and selective plasma technologies;
 - materials for printing technologies;
 - colours and colour metrics.

BIBLIOGRAFIJA

- 21 izvirnih znanstvenih člankov
- 1 kratki znanstveni prispevek
- 1 strokovni članek
- 2 poljudna članka
- 1 samostojni znanstveni sestavek v monografiji
- 2 recenzija, prikaz knjige, kritika
- 1 intervju
- 9 drugo učno gradivo
- 3 objavljeni znanstveni prispevki na konferencah (vabljeni predavanja)
- 11 objavljenih znanstvenih prispevkov na konferencah

BIBLIOGRAPHY

- 21 Original Scientific Articles
- 1 Short Scientific Article
- 1 Professional Article
- 2 Popular Articles
- 1 Independent Scientific Component Part in Monograph
- 2 Review, Book Review, Critique
- 1 Interview
- 9 Other Educational Material
- 3 Published Scientific Conference Contributions (Invited Lecture)
- 11 Published Scientific Conference Contributions
- 21 Published Scientific Conference Contribution Abstracts



SLIKA 1:

Nastanek vodnih kapljic na hidrofobni tanki plasti, pripravljene na osnovi funkcionaliziranega poliedričnega oligomernega silseskvioksana (POSS).

FIGURE 1:

Formation of water drops on a hydrophobic thin layer, prepared on the basis of functionalized polyhedral oligomeric silsesquioxane (POSS).

- 21 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 1 patentna prijava
- 3 predavanja na tujih univerzah
- 1 končno poročilo o rezultatih raziskav
- 3 elaborat, predštudija, študija
- 4 diplome
- 2 doktorata

GLAVNI DOSEŽKI V LETU 2007

- V letu 2007 smo intenzivno nadaljevali z raziskovanjem oligofunkcionaliziranih poliedričnih silseskvioksanov (POSS), sintetiziranih na osnovi bazične hidrolize. Pripravili smo mono-, di- in trifunkcionalizirane ($R_xR_yR_z''(SiO_{3/2})_8$, $x+y+z = 6, 8, 10, 12, \dots$) POSS materiale s fenilnimi, izooktilnimi, akrilnimi, amino, perfluoro in merkaptoskupinami. Preliminarni testi so pokazali, da

- 1 Published Professional Conference Contribution Abstract
- 1 Patent Application
- 3 Invited Lectures at Foreign Universities
- 1 Final Research Report
- 3 Treatise, Preliminary Study, Study
- 4 Undergraduate Theses
- 2 Doctoral Dissertations

IMPORTANT ACHIEVEMENTS IN 2007

- In year 2007 we intensively continued with our investigation of oligofunctionalised polyhedral silsesquioxanes (POSS), synthesised using basic hydrolysis. Mono-, di- and trifunctionalised POSS materials ($R_xR_yR_z''(SiO_{3/2})_8$, $x+y+z = 6, 8, 10, 12, \dots$) with phenyl, isooctyl, acrylic, amino, perfluoro and mercapto groups were prepared. Preliminary tests revealed that introduction of various organic groups in POSS species significantly influence their hydro-



SLIKA 2:

Paneli za sončne zbiralnike, ki so bili izdelani v okviru projekta SEONES, ki smo ga izvajali za Trimo, d.d., Trebnje.

FIGURE 2:

Panels for solar collectors prepared in the frame of SEONES project of Trimo d.d., Trebnje, Slovenia.

lahko z uvajanjem različnih organskih skupin v POSS strukture močno povečamo njihove hidrofobne in oleofobne lastnosti (Slika 1). Demonstrirali smo tudi uporabnost POSS materiala, funkcionaliziranega z izooktilnimi in amino skupinami za protikorozijske zaščitne prevleke na aluminijevi zlitini AA 2024, ki se veliko uporablja v letalski industriji. S tem smo nadgradili raziskave protikorozijskih zaščitnih prevlek na osnovi urea/poli(dimetilsiloksanskega) sol-gel hibridnega prekursorja. Naše raziskave protikorozijskih zaščitnih prevlek so prispevale k pridobitvi novega CRP projekta MORS z naslovom *Priprava in karakterizacija hibridnih, nanostrukturiranih premazov za korozijsko zaščito kovinskih površin* (M1-0238) skupaj z Zavodom za gradbeništvo, Ljubljana in Colorjem d.d., Medvode.

- Uspešno smo zaključili EU projekt Solabs v okviru katerega smo razvijali spektralno selektivne barvne premaze, neodvisne od debeline apliciranega nanosa (Thickness Insensitive Spectrally Selective (TISS) coatings), ki so namenjeni uporabi v kolektorskih sistemih na fasadah stavb. Izkušnje, ki smo jih pridobili v okviru tega projekta, so pokazale, da so tehnološki parametri pri pripravi TISS barv zelo pomembni (temperatura, porazdelitev velikosti delcev, vrstni red dodajanja pigmentov in aditivov v barvno formulacijo,...), prav tako pa tudi parametri, ki vplivajo na nanašanje TISS premaza (vsebnost topila in njegova kemijska narava, kot brizganja,...). Začeli smo tudi z razvojem TISS barvnih premazov, v katerih smo kot dodatke uporabili različne silane oz. že sintetizirane in različno funkcionalizirane POSS materiale. Ti dodatki so močno izboljšali predvsem hidrofobne lastnosti (kontaktni kot $> 140^\circ$) barvnih premazov in kot nagiba, pri katerem je stekla vodna kapljica, se je zmanjšal $< 10^\circ$. Na ta način se močno izboljša »easy-to-clean« učinek, saj vodne kapljice zdrsnejo s površine in s seboj odnesejo vso umazanijo. Dodajanje ustreznih modificiranih

phobicity and oleophobicity (Figure 1). The promising application of POSS material functionalised with isooctyl and amino groups for corrosion protective coatings of aluminium AA 2024 alloy was demonstrated. With this topic we upgraded our investigation of corrosion protective coatings on the basis of urea/poly(dimethylsiloxane) sol-gel hybrid precursor. The mentioned investigations contributed to our participation in a new CRP project entitled *Preparation and characterisation of hybrid, nanostructured coatings for corrosion protection of metal surfaces* (M1-0238) together with Slovenian National Building and Civil Engineering Institute, Ljubljana, Slovenia and Color, d.d., Medvode, Slovenia.

- The EU project Solabs, in the frame of which we developed Thickness Insensitive Spectrally Selective (TISS) coloured paint coatings for solar façades, was successfully finished. The experiences gathered in this project revealed the importance of the technological parameters (temperature, particle size distribution, order of addition of pigments and additives in paint formulation,...) for the preparation of TISS paints, as well the importance of conditions of paint spraying (solvent content and its chemical nature, angle of spraying,...). We also started the development of TISS paints with added silanes or variously functionalised POSS materials. These additives significantly improved the hydrophobic properties (contact angle $> 140^\circ$) of paint coatings and consequently, the sliding angle for water decreased to $< 10^\circ$. In this way we increased the »easy-to-clean« effect, the water drops slipped from the surface and sweep away the dirt. However, the addition of appropriately modified POSS additives that express the hydrophobic and oleophobic properties at the same time, will contribute also to the improvement of oleophobic properties of coloured surfaces and therefore, to prevention of the contamination of façades with exhaust gases from vehicles (transport) or



SLIKA 3:

V letu 2007 je potekala obnova študentske sobe, v kateri je svoje mesto dobil novi in sodobno opremljeni laboratorij L02.

POSS aditivov, ki istočasno izražajo hidrofobne in oleofobne lastnosti, pa bo znatno pripomoglo tudi k povečanju oleofobnih lastnosti barvnih površin in s tem k preprečevanju onesnaženja fasad z izpušnimi plini in izpusti iz dimnikov. Spektralno selektivne barve smo razvijali tudi v okviru industrijskega projekta *SEONES, Barvni selektivni – energetska učinkoviti premazi za elemente ovojja nizkoenergijskih stavb* za Trimco d.d., Trebnje (Slika 2).

- Raziskave površin pigmentiranih premazov so pokazale, da je videz teh površin odvisen od mikroskopske oblike površine. Dokazali smo, da poleg povprečne hrapavosti, ki je določena s povprečno višino površinskih nepravilnosti, na videz površine močno vpliva tudi povprečna razdalja med površinskimi nepravilnostmi. Ti rezultati so pomembni za načrtno spreminjanje lastnosti, ki vplivajo na videz površin. Najosnovnejša med njimi je stopnja sijaja ali mat efekta.
- Analizirali smo osnovne lastnosti svetlobno občutljivega polimera na epoksi osnovi. Gre za relativno nov UV-fotorezist, ki se zaradi svojih odličnih lastnosti že uporablja v sodobni tehnologiji mikromašininga. Ta material smo

FIGURE 3:

In 2007 we started the renovation of the student room into a new and up-to-date laboratory.

fumes from chimneys (heating). Spectrally selective paints were developed also in the frame of industrial project *SEONES, Coloured selective – energy effective coatings for façade elements for low-energy consumption buildings* for Trimco, d.d., Trebnje, Slovenia (Figure 2).

- Investigations of the surfaces of pigmented coatings revealed that their appearance depended on the microscopic properties of their surfaces. It is not only the mean high of the surface irregularities that define the level of surface gloss but also the mean distance between them. Our research results are important for successful engineering of surface appearance attributes, most important for level of surface gloss.
- Basic properties of light-sensitive epoxy-based polymer were analysed. Excellent properties of the relatively novel UV-photoresist were approved what enables its use in micro-machining technology applications. This material was applied for matrix of nanocomposites with variable electrical conductivity. It was shown that it is a suitable sensing material for chemical vapour sensors.
- Colorimetric methods were applied together with methods of classical optics for

- uporabili za matriko kompozita z variabilno prevodnostjo in pokazali, da ga je mogoče uspešno uporabiti za senzorski material v različnih kemijskih senzorjih.
- Z uporabo metod barvne metrike v kombinaciji z metodami klasične optike smo analizirali nekaj efektivnih tiskarskih barv. Prav tako smo pričeli s prvimi raziskavami lastnosti materialov, ki se uporabljajo pri različnih metodah tiska in lastnosti potiskanih izdelkov.
 - Nadaljevali smo tudi z raziskavami interkalacijskih tankih plasti (CeVO_4 , V_2O_5 , CeO_2 , Ce/Ti-oksidi,...) za nasprotno elektrodo v elektrokromnih (EC) sklopih ter s pripravo elektrolitov na osnovi kondenziranih ionskih tekočin za te sklope. EC sklop, ki smo ga pripravili skupaj s skupino italijanskih raziskovalcev z Univerze v Rimu »La Sapienza«, v katerem smo med tanki plasti nanokristaliničnega WO_3 in V_2O_5 aplicirali ionsko tekočino n-butyl-n-metilpirolidinijev bis(trifluorometansulfonil)imid, imobilizirano v polietilenoksidni polimerni matriki, se je izkazal po stabilnosti odziva in optično modulacijo ($\Delta T \sim 50\%$ pri 650 nm). Radi bi še poudarili, da je dr. Vasko Jovanovski, ki je pripravil doktorsko disertacijo o elektrolitih za EC sklope in Grätzlove fotoelektrokemijske celice, prejel Preglovo nagrado Kemijskega inštituta za izjemno doktorsko delo.
 - V okviru EU projekta Apollon-B (nosilec: dr. Stanko Hočevar) smo po sol-gel postopkih pripravili nove protonsko prevodne membrane. Za pripravo teh membran smo sintetizirali nekaj novih sol-gel prekurzorjev, ki membranam podelijo fleksibilnost in temperaturno obstojnost.
 - V sodelovanju z Laboratorijem za biotehnologijo smo začeli uporabljati silane kot povezovalce med osnovo (steklom, polimeri) in bakterijskim peptidom polimiksinom B. Prvi rezultati kažejo dobro redukcijo rasti bakterij na takšni površini. Cilj te raziskave je uporaba teh prevlek na medicinskih pripomočkih (katetri).
- analysis of some effect printing inks. The research of materials used in modern digital printing technologies was also started.
- Investigations of thin films with intercalation properties (CeVO_4 , V_2O_5 , CeO_2 , Ce/Ti-oxide,...) for counter electrodes in electrochromic (EC) devices were continued, as well the preparation of electrolytes on the basis of condensed ionic liquids. EC device prepared together with the Italian group of researchers from the University of Rome "La Sapienza", in which we applied an ionic liquid n-butyl-n-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide in a polyethyleneoxide matrix in between the thin nanocrystalline films of WO_3 and V_2O_5 , distinguished with its response stability and optical modulation ($\Delta T \sim 50\%$ at 650 nm). In addition, we would like to stress that dr. Vasko Jovanovski was awarded with the Pregl prize of the National Institute of Chemistry for an exceptional Ph.D. dissertation for his work on electrolytes for EC and Grätzel photoelectrochemical cells.
 - In the frame of EU project Apollon-B (responsible at NIC: Dr. Stanko Hočevar) we prepared new proton conducting sol-gel membranes. For their preparation we synthesised some new sol-gel precursors that impart flexibility and temperature stability to the membranes.
 - In collaboration with the Laboratory of Biotechnology we started to use silanes as linkers between the base (glass, polymers) and the bactericidal peptide polymyxin B. First results showed good reduction in bacteria growth on such a surface. The aim of this investigation is the use of these coatings on the medical instruments (catheters).
 - With the Laboratory for Polymer Chemistry and Technology we intensively collaborated on the preparation and the characterisation of copper oxides with polyol method. It was shown that it is possible to prepare Cu_2O nano wires with polyol method without any stabilisers or other additives. However, we have to stress that the final morphology of

- Z Laboratorijem za polimerno kemijo in tehnologijo smo intenzivno sodelovali pri pripravi in karakterizaciji bakrovih oksidov s poliolno metodo. Pokazali smo tudi, da je možno pripraviti Cu_2O nano žičke s poliolno metodo brez kakršnihkoli stabilizatorjev ali drugih dodatkov. Poudariti pa moramo, da je končna morfologija Cu_2O nano žičk odvisna od koncentracije začetnega prekursorja in pogojev sinteze.
- Proti koncu leta smo pričeli s prenovo študijske sobe S-208 in jo preuredili v nov in sodoben laboratorij (Slika 3). S tem smo povečali število laboratorijskih prostorov v L02, kar bo pripomoglo h kakovostnejšemu delu.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Color d.d., Medvode; razvoj premazov za sončne zbiralnike in fasade (sodelovanje v okviru Solabs EU projekta, SEONES projekta in CRP MORS projekta);
- Fotona d.d., Ljubljana; razvoj nizkoemitivnih kamuflažnih premazov za tanke (sodelovanje v okviru CRP MORS projekta);
- Trimoterm d.d., Trebnje; Barvni selektivni – energetsko učinkoviti premazi za »Solarni panel Trimoterm« (sodelovanje v okviru projekta SEONES - Razvoj sistemov za nizkoenergijske stavbe, 2006-2007);
- Univerza v Ljubljani, Naravoslovnotehniška fakulteta in Tekstina, tekstilna industrija Ajdovščina, d.d.; razvoj večfunkcionalne zaščitne tekstilije za vojaške uniforme (sodelovanje v okviru samostojnega projekta MORS);
- Center odličnosti »Nanoznanosti in nanotehnologije« (CO NIN – RPR), Nanomateriali v elektrokemijskih sistemih.

MEDNARODNO SODELOVANJE

- Development of unglazed solar absorbers (resorting to coloured selective coatings on steel material) for building facades and integra-

Cu_2O nano wires depend on concentration of precursor and synthesis conditions.

- At the end of the year we started with the renovation of the student room S-208 and we remake it in a new and contemporary laboratory (Figure 3). With this action we increased the laboratory facilities in L02, which will significantly contribute to an improvement of working conditions.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Color d.d., Medvode, Slovenia; development of paint coatings for solar collectors and façades (cooperation in the frame of Solabs EU project, SEONES industrial project and CRP MORS project);
- Fotona d.d., Ljubljana, Slovenia; development of low-emittance camouflage coatings for tanks (cooperation in the frame of CRP MORS project);
- Trimoterm d.d., Trebnje, Slovenia; Coloured selective – energy efficient coatings for »Solar panel Trimoterm« (cooperation in the frame of project SEONES – *Coloured selective – energy effective coatings for façade elements for low-energy consumption buildings*, 2006-2007);
- University of Ljubljana, Faculty of Natural Sciences and Engineering and Tekstina, textile industry Ajdovščina, d.d., Slovenia; development of multifunctional protective coatings for textile for military uniforms (cooperation in the frame of CRP MORS project);
- Centre of excellence »Nanoscience and nanotechnology« (CO NIN – RPR), Nanomaterials in electrochemical systems.

INTERNATIONAL COLLABORATION

- Development of unglazed solar absorbers (resorting to coloured selective coatings on steel material) for building facades and integration into heating systems (SOLABS), Contract N° ENK6-CT-2002-00679, RTD project, 1.1.2003-30.6.2006 (Dr. Boris Orel);

- tion into heating systems (SOLABS), Št. pogodbe N° ENK6-CT-2002-00679, RTD projekt, 1.1.2003-30.6.2006 (dr. Boris Orel);
- Polymer Electrolytes and Non Noble Metal Electrocatalysts for High Temperature Fuel Cells (APOLLON-B), STREP EU projekt, 1. 10. 2006 – 30. 9. 2009 (nosilec: dr. Stanko Hočevar);
 - Polymeric Materials for Solar Thermal Applications, International Energy Agency (IAE), sprejet projekt (december 2005), prošnja za pridruženo sodelovanje;
 - Mreža odličnosti: Nanostructured and Functional Polymer-based materials and Nanocomposites, Proposal No. NOE 500361-2 (dr. Zorica Crnjak Orel);
 - Priprava in karakterizacija uniformnih delcev, bilateralno sodelovanje Slovenija-USA, Clarkson University (dr. Zorica Crnjak-Orel);
 - Študij strukturnih lastnosti sol-gel materialov z nizko emitivnostjo z IR spektroskopijo, bilateralno sodelovanje Slovenija-Indija, 10. 10. 2006 – 31. 12. 2007, Central Glass & Ceramic Research Institute, Sol-Gel Division, Kolkata (dr. Angela Šurca Vuk);
 - Sinteze mešanih sistemov na osnovi titanovega oksida: strukturne, elektrokemijske in površinske lastnosti, bilateralno sodelovanje Slovenija-Italija, 1. 3. 2006 – 31. 2. 2009, University of Trento, Trento (dr. Angela Šurca Vuk);
 - Dinamika protonov v kratkih vodikovih vezeh dihidrata oksalne kisline in sorodnih sistemov – študij z infrardečo disperzijsko analizo, bilateralno sodelovanje Slovenija-Makedonija, Faculty of natural sciences and mathematics, Skopje (dr. Marta Klanjšek Gunde);
 - CIE, Division 1 (dr. Marta Klanjšek Gunde, uradna članica – predstavnica Slovenije);
 - CIE, Division 2, TC2-53, Multi-geometry color measurements of effect materials (dr. Marta Klanjšek Gunde, članica);
 - CIE, Division 1, TC1-66, Indoor daylight illuminant (dr. Marta Klanjšek-Gunde, članica).
- Polymer Electrolytes and Non Noble Metal Electrocatalysts for High Temperature Fuel Cells (APOLLON-B), STREP EU project, 1. 10. 2006 – 30. 9. 2009 (responsible: Dr. Stanko Hočevar);
 - Polymeric Materials for Solar Thermal Applications, International Energy Agency (IAE), Solar Heating and Cooling Programme, Task 39;
 - Network of Excellence: Nanostructured and Functional Polymer-based materials and Nanocomposites, Proposal N°. NOE 500361-2 (Dr. Zorica Crnjak Orel);
 - Preparation and characterisation of uniform particles, Bilateral cooperation Slovenia-USA, Clarkson University (Dr. Zorica Crnjak Orel);
 - Study of structural properties of sol-gel materials with low emissivity using IR spectroscopy, Bilateral cooperation Slovenia-India, 10. 10. 2006 – 31. 12. 2007, Central Glass & Ceramic Research Institute, Sol-Gel Division, Kolkata (Dr. Angela Šurca Vuk);
 - Synthesis of mixed systems on the basis of titanium oxide: structural, electrochemical and surface properties, Bilateral cooperation Slovenia-Italy, 1. 3. 2006 – 31. 2. 2009, University of Trento, Trento (Dr. Angela Šurca Vuk);
 - Dynamics of protons in short hydrogen bonds of oxalic acid dihydrate and related systems – study with infrared dispersive analysis, Bilateral cooperation Macedonia-Slovenia, Faculty of natural sciences and mathematics, Skopje (Dr. Marta Klanjšek Gunde);
 - CIE, Division 1 (Dr. Marta Klanjšek Gunde, official member – representative of Slovenia);
 - CIE, Division 2, TC2-53, Multi-geometry color measurements of effect materials (Dr. Marta Klanjšek Gunde, member);
 - CIE, Division 1, TC1-66, Indoor daylight illuminant (Dr. Marta Klanjšek-Gunde, member).
- MAJOR EQUIPMENT**
- FT-IR spectrometer Bruker IFS 66/S

POMEMBNI INŠTRUMENTI IN OPREMA

- FT-IR spektrometer Bruker IFS 66/S
- FT-IR in FT-Raman spektrometer Perkin Elmer 2000
- Spektrometer Lambda 950 UV/VIS/NIR
- Hewlett-Packard 8453 UV-VIS spektrofotometer z diodnim nizom
- AUTOLAB PGSTAT30 in EG&G PAR 273 potenciostat/galvanostat
- DISPERMAT CN10-F2, VMA-GETZMANN GMBH

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Vasko Jovanovski: Priprava elektrolitov na osnovi ionskih tekočin in njihova uporaba v fotoelektrokemijskih celicah, doktorska disertacija;
- Jelica Vince: Strukturne in spektroskopske lastnosti po sol-gel postopkih narejenih protonsko prevodnih membran, doktorska disertacija;
- Peter Podbršček: Priprava in karakterizacija kompozitnega materiala na osnovi bakra in cinkovega oksida, diplomsko delo;
- Žveglič Maša: Prednosti in omejitve digitalnih tehnologij tiska, diplomsko delo;
- Andreja Jelen: Vpliv efektnih pigmentov na orientacijo odbite in sipane svetlobe, diplomsko delo;
- Roman Kunič: Načrtovanje vrednotenja vpliva pospešenega staranja bitumenskih trakov na konstrukcijske sklope, doktorska disertacija;
- Eva Šimunič: Priprava in uporaba nanokompozitov z metakriloksiipiltrimetoksisilanom, diplomsko delo;
- Piere Guillaume (Polytech' Grenoble, Joseph Fourier University, Francija), 3,5 mesečno delo v L02 v okviru izmenjave Erasmus;
- Quentin Fabrh (Polytech' Grenoble, Joseph Fourier University, Francija), 3,5 mesečno delo v L02 v okviru izmenjave Erasmus.

- FT-IR and FT-Raman spectrometer Perkin Elmer 2000
- Spectrometer Lambda 950 UV/VIS/NIR
- Hewlett-Packard diode array 8453 UV-VIS spectrophotometer
- AUTOLAB PGSTAT30 and EG&G PAR 273 potentiostat/galvanostat
- DISPERMAT CN10-F2, VMA-GETZMANN GMBH

EDUCATION AND IMPORTANT VISITS

- Vasko Jovanovski: Preparation of electrolytes on the basis of ionic liquids and their application in photoelectrochemical cells, Ph.D. dissertation;
- Jelica Vince: Structural and spectroscopic properties of proton conductive membranes prepared using sol-gel routes, Ph.D. dissertation;
- Peter Podbršček: Preparation and characterization of composite material on the basis of copper and zinc oxide, B.S. thesis;
- Žveglič Maša: Advantages and limitations of digital printing techniques, B.S. thesis;
- Andreja Jelen: The influence of effect pigments on the orientation of reflected and scattered light, B.S. thesis;
- Roman Kunič: Assessment of influence of accelerated ageing of bitumen straps on construction joints, Ph.D. dissertation;
- Eva Šimunič: Preparation and use of nanocomposites with metachryloxypropyltrimethoxysilane, B.S. thesis;
- Piere Guillaume, Polytech' Grenoble, Joseph Fourier University, France: 3.5 months work in L02 in the frame of Erasmus student exchange;
- Quentin Fabrh, Polytech' Grenoble, Joseph Fourier University, France: 3.5 months work in L02 in the frame of Erasmus student exchange.

L03

Laboratorij za kemometrijo

Laboratory of Chemometrics



VODJA / HEAD
dr. Marjana Novič

RAZISKOVALCI / RESEARCHERS

dr. Marjan Vračko
dr. Neva Grošelj
dr. Marjan Tušar
dr. Natalja Fjodorova
dr. Milan Randić (4 mesece / months)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

mag. Špela Župerl
Viktor Drgan
Nikola Minovski

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

dr. Sylwester Mazurek (1 mesec / month)
dr. Jaroslaw Panek (12 mesecev / months)
dr. Igor Kuzmanovski (9 mesecev / months)



PODROČJA DEJAVNOSTI

- Uvajanje kemometrije, to je uporabe široke palete matematičnih, statističnih in računalniških metod za reševanje kemijskih problemov, v raziskovalno in razvojno prakso;
- modeliranje kemijskih lastnosti in procesov na področju QSAR študij in iz podatkov, ki jih dobimo s sklopljenimi analiznimi tehnikami;
- uveljavljanje metod umetnih nevronske mreže v kemiji; študij strategij učenja nevronske mreže in razvijanje ustreznih računalniških programov;
- raziskave na področju matematične kemije: uporaba diskretne matematike v strukturalni kemiji, v QSAR študijah, v proteomiki in genomiki;
- študij algoritmov in razvoj programskih paketov;
- uporaba kemometričnih metod v analizi kemiji: zagotavljanje in kontrola kakovosti (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, to the applicative, research, and control laboratories;
- Modelling of chemical properties and processes to 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 chemometrics 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 dodiplomskem in podiplomskem nivoju;
 - izobraževanje na področju metod umetne inteligence in kemometrije v sodelovanju s Fakulteto za kmetijstvo Univerze v Mariboru;
 - 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 Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia on the pre- and postgraduate levels;
 - Education in methods of artificial intelligence and chemometrics in collaboration with Faculty of Agriculture, University of Maribor, Slovenia;
 - 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

- 12 izvirnih znanstvenih člankov
- 2 strokovna članka
- 1 samostojni znanstveni sestavek v monografiji
- 2 objavljena strokovna prispevka na konferencah
- 30 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzetek strokovnega prispevka na konferenci
- 1 predavanje na tuji univerzi
- 1 prispevek na konferenci brez natisa
- 1 vabljeni predavanje na konferenci brez natisa
- 2 doktorata

DOSEŽKI V LETU 2007

- V letu 2007 smo sodelavci Laboratorija za kemometrijo rezultate raziskav predstavili v 10 izvirnih znanstvenih člankih in enem poglavju v monografiji, o svojem delu smo poročali v 30 prispevkih na mednarodnih znanstvenih konferencah in v treh prispevkih na strokovnih konferencah. Sodelujemo z več tujimi univerzami, med drugim smo del raziskav kemometrijskih metod, ki jih razvijamo, predstavili s predavanjem na univerzi Milano Bicocca, Italija. Vsebinska objavljenih del izkazuje dosežke na področju,

BIBLIOGRAPHY

- 12 Original Scientific Articles
- 2 Professional Articles
- 1 Independent Scientific Component Part in Monograph
- 2 Published Professional Conference Contributions
- 30 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 1 Invited Lecture at Foreign University
- 1 Unpublished Conference Contribution
- 1 Unpublished Invited Conference Lecture
- 2 Doctoral Dissertations

ACHIEVEMENTS IN 2007

- In 2007 the research work of the researchers from the Laboratory of chemometrics is represented in 10 original scientific papers, in one book chapter, and in 30 contributions at international scientific conferences and in three contributions at professional conferences. We collaborate with several universities; among others we presented our research on the development of chemometrics meth-

definiranem v raziskovalnem programu *Modeliranje relacij med kemijsko strukturo in lastnostjo snovi - QSAR – QSPR*.

- Profesor Milan Randić, dolgoletni zunanji sodelavec L03 in raziskovalec na raziskovalnem programu *Modeliranje relacij med kemijsko strukturo in lastnostjo snovi - QSAR – QSPR*, je postal častni član Kemijskega inštituta. Naziv mu je ob 60. obletnici ustanovitve Kemijskega inštituta podelil direktor na slovesni prireditvi 27. septembra 2007.
- IBAAC (An Integrated Biomimetic Approach to Asymmetric Catalysis), evropski projekt v okviru Marie Curie Network smo nadaljevali z dvema po-doktorskima raziskovalcema. Ostali so praktično delo, ki so ga izvajali v našem laboratoriju, že zaključili in z njimi dokončujemo zadnje publikacije. Cilj našega sodelovanja je optimizacija katalizatorjev za asimetrično kemijsko sintezo v okolju, ki simulira biološkega. Tako okolje so npr. proteini (streptavidin ali avidin) ali dendrimeri, katerih osnovne enote so aminokisljine. O rezultatih smo poročali na sestanku IBAAC projekta v Muelheimu in na konferenci v Novi Gorici (Spektroskopija v teoriji in praksi).
- Evropski projekt TRACE, ki je bil zastavljen kot integriran projekt od vzorčevanja zemlje in hrane do kemijske analize in statistične obdelave podatkov (v tem delu je vključena tudi naša skupina), je v letu 2007 dokaj uspešno zaključil z zbiranjem podatkov. Tako smo dobili v obdelavo kar nekaj podatkovnih nizov, s pomočjo katerih smo dopolnili in testirali orodje na osnovi umetnih nevronske mreže v MATLAB okolju (TRACE_ANN). O rezultatih smo poročali na sestankih TRACE projekta v Ljubljani, Katowicah in na Kreti, Grčija, ter na konferencah v Mariboru (Slovenski kemijski dnevi) in na Finskem (10. skandinavski kemometrijski simpozij). Da bi predstavili razvito programsko orodje TRACE_ST, smo v okviru WP6 partnerjev projekta organizirali dvodnevno delavnico v

ods at the University Milano Bicocca, Italy. The content of published papers shows the achievements in the field defined in the research program *“Modelling of structure–property relationships – QSAR–QSPR”*.

- Professor Milan Randić, a member of the L03 chemometrics research team for a long time, and a collaborator on the research program *“Modelling of structure–property relationships – QSAR–QSPR”* became an honourable member of the National Institute of Chemistry. The title was awarded by the director at the 60th anniversary of the Institute at the ceremony on September 27th.
- IBAAC (An Integrated Biomimetic Approach to Asymmetric Catalysis), European project in the Marie Curie Training Network scheme was accomplished with two post-doctoral researchers. All other fellows had finished the practical work in our laboratory and in 2007 we were completing their results to be published. The goal of the chemometrics contribution to the project is to optimize the catalysts for asymmetric chemical synthesis in the environment mimicking the biological systems, for example proteins (streptavidin, avidin) or dendrimers of amino acid units. We reported the results at internal IBAAC conference in Muelheim, Germany and in Nova Gorica, Slovenia at the 15th International Symposium Spectroscopy in Theory and Practice.
- The European project TRACE, which is an integrated project aimed to collect and analyse samples of soil and food commodities (our group was included for statistical analysis of collected data) in 2007 practically accomplished the data collection. So we have several data sets available, which were exploited to complete and test the neural networks based tool in Matlab environment (TRACE_ANN). The results were reported at the internal TRACE meetings in Ljubljana, Slovenia, Katowice, Poland and in the annual TRACE conference at Crete, Greece. Besides some results were presented at the meeting

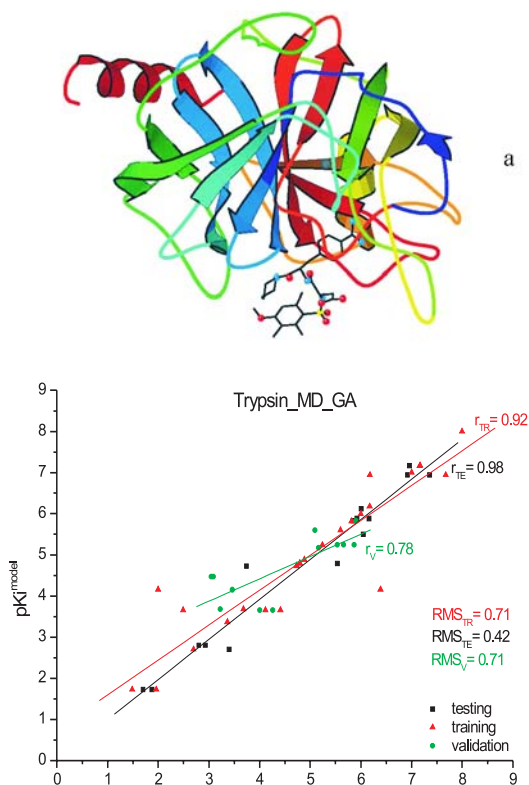
- Nijmegen-u na Nizozemskem. Partnerjem WP1 in WP2 smo s teoretično predstavitvijo in praktičnim tečajem približali uporabo programskega paketa na konkretnih primerih.
- Nadaljevali smo delo na evropskem projektu CAESAR (Computer-Assisted Evaluation of industrial chemical Substances According to Regulations). Poleg podatkovne baze karcinogenih spojin (806 spojin) je naša skupina pripravila tudi primerjalno študijo predpisov in meril za oceno toksičnosti v EU, Rusiji in v članicah OECD. Podatkovni niz spojin s poznanimi kemijskimi strukturami in določeno stopnjo karcinogenosti je bil izbran iz raznih javno dostopnih virov. O rezultatih smo poročali na konferencah v Novi Gorici (Spektroskopija v teoriji in praksi), v Portu na Portugalskem (SETAC) in na internih CAESAR srečanjih v Ljubljani in v Liverpoolu, Velika Britanija.
 - Nadaljevali smo z delom na industrijskem projektu s podjetjem IMS-ADITOIL d.o.o., Trzin; pogodba št. 120/06-L03 o dolgoročnem sodelovanju na področju raziskav in razvoja nizko temperaturnih bitumnov in asfaltnih zmesih. V okviru pogodbe sodelavci kemijskega inštituta opravljamo temeljne in aplikativne raziskave, razvijamo analitske metode, pripravljamo ekspertna mnenja, pripravljamo skupaj z IMS-ADITOIL d.o.o. projekte in predstavitve za strokovno javnost o nizko temperaturnih bitumnih in asfaltnih zmesih. V letu 2007 smo o delu poročali na konferencah v Budimpešti, Madžarska (Chemometrica 2007), v Novi Gorici (Spektroskopija v teoriji in praksi), ter na strokovnih konferencah v Ljubljani in Kranjski gori (Združenje asfalterjev Slovenije).
 - Z Univerzo v Trstu, Italija (Biophysics and Macromolecular Chemistry BBCM) imamo sporazum o dolgoročnem sodelovanju. Sporazum temelji na skupnih raziskovalnih interesih Oddelka za biokemijo, biofiziko in of Slovenian Chemical Society in Maribor, Slovenia (Slovenski kemijski dnevi) and in Finland (10th Scandinavian Chemometrics Symposium). In order to demonstrate the developed program tool TRACE_ST chemometrics tool (TRACE_ANN is one part of it), we organised within the WP6 group two-day workshop in Nijmegen, the Netherlands. With the theoretical and practical (hands-on) demonstrations on the examples from TRACE data sets we explained to the WP1 and WP2 partners (experimentalists) how to use and exploit the developed chemometrics program package.
 - We continued the work on EU project CAESAR (Computer-Assisted Evaluation of industrial chemical Substances According to Regulations). In addition to the compilation of carcinogenicity data set (806 compounds) the contribution of our group was a comparative study of regulations and measures for assessment of toxicity in EU, Russia, and OECD member states. The data set with given chemical structures and carcinogenicity data was compiled from several public available sources. We have reported about the initial achievements in Nova Gorica, Slovenia at the 15th International Symposium Spectroscopy in Theory and Practice, in Porto (SETAC meeting in Portuguese) and at internal CAESAR meetings in Ljubljana, Slovenia and Liverpool, Great Britain.
 - In the frame of the industrial project with IMS-ADITOIL d.o.o., Trzin, Slovenia contract no. 120/06-L03 about long-term collaboration in the field of research and development of low-temperature bitumen and asphalt mix. We perform basic and applicative research, develop analytical methodology, we prepare expert opinions and together with IMS-ADITOIL d.o.o. we prepare projects and presentations about low temperature bitumen and asphalt mix for professional public meetings. In 2007 we have reported about the

makromolekularno kemijo Univerze v Trstu (profesorica dr. Sabina Passamonti) in Laboratorija za kemometrijo KI (dr. Marjana Novič). Tudi v letu 2007 smo na osnovi skupnih raziskav poročali na konferencah (CMTPI v Moskvi, Rusija, ISSTP v Novi Gorici in na konferenci v Saarbruecken-u v Nemčiji). Mlada raziskovalka Špela Župerl na osnovi rezultatov skupnih raziskav pripravlja doktorsko disertacijo.

- Pod mentorstvom naših sodelavcev in v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani je en mladi raziskovalec začel z delom, dva pa sta

results in Budapest, Hungary (Chemometrica 2007), in Nova Gorica, Slovenia (15th International Symposium Spectroscopy in Theory and Practice), and at technical conferences in Ljubljana and Kranjska gora (Slovenian Asphalt Pavement Association).

- We have a formal agreement with the University of Trieste, Italy (Biophysics and Macromolecular Chemistry BBCM) about a long-term collaboration. The agreement is based on the common research interests between the group of prof. S. Passamonti and our laboratory. In 2007 we reported on common research results at a Scientific confer-



SLIKA 1:

Kompleks inhibitorja in tripsina (PDB ID=1K1N) z ligandom, vidnim na dnu slike (a); Regresijska premica med eksperimentalnimi in napovedanimi vrednostmi pKi, dobljenimi s pomočjo modela protitočne nevronske mreže 59 peptidomimetičnih molekul za reduciran niz spremenljivk – molekularskih deskriptorjev (b).

FIGURE 1:

Inhibitor-trypsin complex (PDB ID=1K1N) with the ligand seen at the bottom of the plot (a); regression plots of the experimental versus predicted pKi obtained by the counter-propagation neural network model for a reduced set of variables based on molecular descriptors of 59 peptidomimetic molecules (b).

nadaljevala doktorsko izobraževanje. Prva mlada raziskovalka je opravila vse študijske obveznosti in zaključuje z raziskovalnim delom, ki ga bo končala po porodniškem dopustu. Drugemu mlademu raziskovalcu je bil na osnovi doseženih rezultatov odobren neposreden prehod na doktorat brez magistriraja, tretji pa je z doktorskim študijem pričel jeseni 2007.

KRATEK OPIS DELA IN REZULTATOV

Glavnina raziskav je bila v letu 2007 utemeljena z raziskovalnim programom P1-017, *Modeliranje relacij med kemijsko strukturo in lastnostjo snovi - QSAR - QSPR*. Zastavljeni raziskovalni program nam omogoča širitev mednarodnih povezav in vključitev v evropske in domače industrijske projekte. Na osnovi računskih modelov, ki popisujejo relacijo med kemijsko strukturo in lastnostjo snovi, lahko prispevamo k oceni strupenosti vseh spojin, ki se sproščajo v okolje, in tako zmanjšamo potrebo po poskusih na živalih. Teste, narejene s pomočjo računskih modelov, imenujemo »in silico«, glede na zahtevnost pa sledijo »in vitro« ter »in vivo« testi. »In vitro« so laboratorijski testi s pomočjo kemijskih in bioloških reagentov, medtem ko za »in vivo« teste potrebujemo testne živali. Poleg tega, da so »in vivo« testi dragi in časovno zamudni, so tudi etično sporni, zlasti ko so v teste vključene živali višjih zvrsti; v veliko državah so testi na določenih živalskih vrstah že prepovedani. Alternativne računalniške metode, tako imenovane QSAR metode (Quantitative Structure - Activity Relationship), so torej zelo obetavne za napovedovanje toksičnosti novih ali biološko še netestiranih spojin, ker so cenejše in hitrejšje od standardnih metod in ne zahtevajo testnih živali. Na tem področju smo v letu 2007 objavili rezultate dela na razvoju modela za napovedovanje aktivnosti nekaterih fenolov kot zaviralcev raka. Pri teh raziskavah je sodeloval indijski partner, ki je bil gostujoči raziskovalec v našem laboratoriju v okviru bilateralnega projekta z Indijo. Med QSAR raziskave, ki so bile končane v lanskem letu, sodijo tudi modeli

ence CMTPI in Moscow, Russia, at ISSTP in Nova Gorica, Slovenia and at a conference in Saarbruecken in Germany. One of our young researchers is preparing the PhD thesis including a part of the obtained results in collaboration with the Italian colleagues.

- We offer mentorship to three PhD students pursuing the PhD studies in our laboratory in agreement with the Faculty of Chemistry and Chemical Technology - University of Ljubljana, Slovenia and Faculty of Pharmacy of the same University. Two of the PhD students already completed all study obligations and they have to continue the research work, while the third one has started in October 2007.

SHORT DESCRIPTION OF RESEARCH AND RESULTS

In 2007 the majority of the research work was accomplished in the financing frame of the research program P1-017, *Modelling of structure-property relationships - QSAR-QSPR*. The core of the research project enables us to extend the international collaborations and to integrate into European and domestic industrial projects. We develop computational models that relate chemical structure with the property of compounds, which enables us to assess toxicity of chemicals released into the environment and thus reduce the need for animal tests. Computational or »in silico« models are usually followed by »in vitro« or »in vivo« models, which are to be reduced. »In vitro« models are based on laboratory tests with chemical and biological reagents, while for the »in vivo« tests we need animals. The latter are time consuming and expensive, besides they are questionable for ethical reasons especially if higher species are included; in many countries the tests on some species are already forbidden. Alternative computational methods, so called QSAR methods (Quantitative Structure - Activity Relationship) are promising for prediction of toxicity of new or biologically not tested existing chemicals, because they are faster and cheaper

za napoved vezavnih konstant med encimom (trombin in tripsin) in peptidom podobnimi majhnimi molekulami.

Pomemben dosežek v letu 2007 je objava rezultatov ovrednotenja strukturne podobnosti proteinov v generičnih zdravilih. To delo je povezano z industrijskim projektom z Lekom, ki je bil zasnovan kot razvoj večstransko podprtega postopka (vključno z eksperimentalno rekombinantno sintezo, spektroskopijo in kemoinformatiko), potrebnega za razvoj in registracijo generičnih zdravil. Zaradi pre zgodnje smrti nosilnega raziskovalca s strani Leka je nadaljevanje projekta negotovo. Naslednji dosežek je plod sodelovanja z

than standard methods and spare the animals. In this field we published the results of our research work in 2007 on the development of a model for prediction of activity of selected phenols as anti-cancer agents. This research was supported also by an Indian partner, who visited our Laboratory in the frame of bilateral project with India. Among the QSAR researches accomplished in 2007 is also a predictive model for trypsin and thrombin binding affinities of small peptidomimetic ligands.

An important achievement in 2007 is a publication of the results about the quantification of structural similarity of proteins in biopharmaceuticals. The research work was initi-



SLIKA 2:
Podelitev naziva častnega člana Kemijskega inštituta profesorju Milanu Randiću

FIGURE 2:
Inauguration of professor Milan Randič, honourable member of the Institute

Zavodom za zdravstveno varstvo Maribor (ZZVMB), in sicer študija kvalitete voda različnih vodnjakov, objavljena 2007.

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

Raziskave na področju teorije grafov prispevajo v QSAR področje nove metode za opis strukture molekul, med njimi tudi proteinov, ki so zaradi svoje specifične narave in velikosti vedno poglavje zase. Na tem področju smo objavili rezultate v štirih publikacijah in poročali v šestih prispevkih na znanstvenih konferencah. Posebno pomembne so raziskave strukturnih reprezentacij proteinov (npr. 2D reprezentacije na osnovi lastnosti gradnikov - aminokislin, ali reprezentacije na osnovi zvezdastih grafov, glej bibliografijo) saj na tem področju še ni na voljo veliko prostih ali komercialnih programskih paketov, ki bi omogočali izračune takih strukturnih deskriptorjev.

Na področju modeliranja kemijskih procesov smo izpopolnili model, s pomočjo katerega lahko študiramo dogajanje na ionsko-izmenjevalni koloni ali napovedujemo rezultate realnih

ated by the industrial project with Lek d.d., Slovenia, joining the experimental recombinant synthesis, spectroscopy, and chemoinformatics needed in the development and registration of biopharmaceuticals. The future of this project is unclear because of premature death of the principal investigator from Lek. The next attainment is an expertise on ground water investigation, the result of our collaboration with the Institute of Public Health Maribor, Slovenia (IPHMB) published in 2007.

The study of membrane protein bilitranslocase (in cooperation with the University of Trieste, Italy) resulted in the explanation of potential mechanism of action of the transport protein. Bilitranslocase is a liver protein, responsible for the transport of bilirubin (and other molecules) through the cell membrane. Our aim was to clarify the mode of interaction of flavonoids with the bilitranslocase. The study showed that binding interaction depends primarily on the formation of hydrogen bonds, which decreases the importance of the old hypothesis about interactions of charged molecular moieties. Special emphasis was given to the selection of structural descriptors in the construction of the models. The results showed that, contrary to anthocyanins, most flavonols (originating from food) did not interact with bilitranslocase, while some aglycones were weakly bounded. Quantitative analysis of the relationship between chemical structure and binding affinities revealed parts of molecules potentially responsible for the binding mechanism between the ligand and the host protein.

The investigations based on graph theory contributed to the QSAR field of the research with new descriptions of chemical structure of molecules including proteins, which ought to have due to their size and specific structure a special treatment. In this area we published four papers and reported at six international scientific conferences. Of special interest are the investigations on the structural representations of proteins (as for example 2D representations on the basis of physico-chemical properties of

meritev (retencijske čase in/ali obliko kromatografskih vrhov). Izpopolnitev algoritma za simulacijo separacijskih procesov v ionsko-izmenjevalni kromatografiji, ki nam omogoča vpogled v časovno in prostorsko porazdelitev koncentracij ionov analita in eluenta na kromatografski koloni, omogoča izračune za vse analite ne glede na kombinacijo nabojev analita in eluenta. Rokopis z rezultati je bil sprejet za objavo v *Journal of Chromatography A*.

Industrijski projekt z IMS-ADITOIL d.o.o., Trzin nadaljujemo z raziskavami o nizko temperaturnih bitumnih in asfaltnih zmesih. V okviru navedene pogodbe smo na Kemijskem Inštitutu v letu 2007 izvedli naslednje dejavnosti: (i) na konferencah v Budimpešti, Madžarska (Conferentia chemometrica 2007) smo predstavili kemometrični pristop k izdelavi asfaltnih receptur ("Counterpropagation neural network as a model for asphalt mix design"); (ii) v Novi Gorici (15. mednarodni simpozij Spektroskopija v teoriji in praksi) smo poročali o vplivu in obstojnosti dodatka asfaltnih zmesi Sasobita ("Recycling ability of asphalts containing low temperature bituminous binders"); (iii) na 11. kolokviju o asfaltnih in bitumnih v Kranjski gori pa smo s predavanjem "Vpeljava kemijskih metod za preverjanje uporabnosti recikliranih bitumnov" predstavili prednosti asfalta z dodatkom Sasobita in uspeli prepričati nekatere izvajalce v gradbeništvu, da bodo te vrste asfalte vgrajevali v cestne odseke nove gorenjske avtoceste; (iv) Na strokovni konferenci v Ljubljani ("Obvezna uporaba novih standardov za asfalt SIST EN 13108 in novosti pri laboratorijskih preiskavah, Novosti pri laboratorijskih preiskavah" na 6. izobraževanju tehničnega asfaltskega kadra) smo predstavili nove evropske standarde za metode preskušanja asfaltov.

V letu 2007 smo v okviru IBAAC EU projekta del kemoinformacijske kompleksne raziskave sistema »Avidin/Streptavidin – biotiniran ligand« dopolnili in pripravili za objavo. Prav tako smo v glavnem zaključili z raziskavo optimiranja

amino acids, or the representations by star-like graphs, see bibliography), because there are not many free or commercially available software packages offering the calculations of such structural descriptors.

In the field of modelling chemical processes we developed and completed a model as a tool enabling the study of distribution of ion concentrations in ion-exchange column, or to make predictions for real measurements (retention times and/or shape of chromatographic peaks). Upgrade of the model and the algorithm for simulation of separation processes in ion-exchange chromatography, which enables us to monitor time-space distribution of analyte and eluent concentrations in chromatographic column, will facilitate the calculations for all analytes regardless the combination of analyte/eluent charges. We reported on the results in the manuscript, which had been accepted for publication in *Journal of Chromatography A*.

We proceed with the industrial project with IMS-ADITOIL directed towards investigation of low temperature bitumen and asphalt mix. In the scope of the long term agreement we have accomplished in 2007 the following: (i) at a conference in Budapest, Hungary (Chemometrica 2007) we have reported on chemometrical approach to asphalt mix recipe ("Counterpropagation neural network as a model for asphalt mix design"); (ii) in Nova Gorica, Slovenia (15th International Symposium Spectroscopy in Theory and Practice) we reported on the influence and stability of the additive to the asphalt mix Sasobit ("Recycling ability of asphalts containing low temperature bituminous binders"); (iii) at 11th Colloquium on Asphalt and Bitumen in 2005 in Kranjska gora, Slovenia we presented a lecture entitled "Introduction of chemical methods for checking the properties of recycled bitumen" in which we demonstrated the advantages of the asphalt mix with Sasobit and we succeeded to persuade some companies that they would build the new asphalt mix with Sasobit into some sections of the new highway in highland region of



SLIKA 3:
Sestanek partnerjev EU projekta CAESAR v Ljubljani,
december 2007

dendrimerov kot okolja za asimetrično katalizo. Rezultati so zbrani in pred objavo čakamo še na eksperimentalno potrditev naših računskih napovedi.

TRACE projekt se nadaljuje z dopolnjevanjem in testiranjem programskega paketa za statistično obdelavo podatkov kemijske sestave tal in hrane. Na dvodnevni delavnici v Nijmegen-u na Nizozemskem smo predstavili razvito programsko orodje TRACE_ST, pri katerem smo odgovorni za klasifikacijo in napovedovanje lastnosti z nevronskimi mrežami. Klasifikacija je večinoma narejena glede na geološko sestavo vzorčenih mest. Ob dotoku novih podatkovnih nizov posameznih vzorcev (zemlja, voda, hrana) sproti dopolnjujemo modele za klasifikacijo vzorcev. Končni cilj je povezava med kemijsko sestavo vzorcev in geološko sestavo področja, kjer so bili vzorci pridobljeni. Na ta način bi lahko hrano opremili z nalepkami s specifikacijo, ki bi dokazovala izvor.

Pri CAESAR projektu smo vsi partnerji zaključili z zbiranjem podatkovnih baz in se sedaj ukvarjamo z optimizacijo napovednih modelov za pet definiranih področij: karcinogenost, mutagenost, teratogenost, kožna občutljivost, bio-akumulacijski faktor. Poleg tega smo v naši skupini naredili primerjalno študijo predpisov in meril za oceno toksičnosti v EU, Rusiji in v članicah OECD, ki smo jo poslali v Journal of Environmental Science and Health Part C-En-

FIGURE 3:
Workshop of partners of EU project CAESAR in
Ljubljana, December 2007

Slovenia; (iv) at a professional conference in Ljubljana, Slovenia, we reported on the new European standards for the methods of asphalt tests.

In 2007 we completed a part of chemoinformatics research of the system »Avidin/Streptavidin – biotinilated ligands« within the IBAAC EU project. The results reported in the manuscript were sent for publication. Also the research work on optimization of dendrimers of amino acids as an environment for the asymmetric catalysis was practically completed. The results of the prediction model for optimization of the dendrimers structure have to be confirmed by the experimentalists before publishing.

Trace EU project is going on with the upgrading and testing the software package for statistical evaluation of data on chemical composition of soil and food commodities. In Nijmegen, the Netherlands, we organised a two-day workshop at which the toolbox TRACE_ST was demonstrated. Our part concerns the neural network tool in Matlab environment for classification and prediction of properties connected to the available data sets (classification was mainly done regarding geology of the sampling sites).

The status at CAESAR EU project is in the final stage of data collection. We started with the modelling for five defined toxicity endpoints: Carcinogenicity, mutagenicity,

vironmental Carcinogenesis & Ecotoxicology Reviews. Članek je bil sprejet v objavo brez popravkov.

SODELOVANJE Z INDUSTRIJO

- IMS-ADITOIL d.o.o., Trzin

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:

- projekt TRACE (FP6-2003-FOOD-2-A) (*Tracing Food Commodities in Europe*). (Contract No. TRACE-IP-006942);
- projekt IBAAC (*An Integrated Biomimetic Approach to Asymmetric Catalysis*) (Contract No. MCRTN –CT-2003-505020);
- projekt CAESAR (*Computer-Assisted Evaluation of industrial chemical Substances According to Regulations*) (SSPI-022674);

teratogenicity, skin sensitization, and bioaccumulation factor. Besides, our group prepared a comparative study of regulations and measures for assessment of toxicity in EU, Russia, and OECD member states. The manuscript was sent to the Journal of Environmental Science and Health Part C-Environmental Carcinogenesis & Ecotoxicology Reviews; it was accepted for publication without changes.

COLLABORATION WITH THE INDUSTRY

- IMS-ADITOIL d.o.o., Trzin, 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:

- Project TRACE (FP6-2003-FOOD-2-A) (*Tracing Food Commodities in Europe*). (Contract No. TRACE-IP-006942);



SLIKA 4:
Delovni sestanek partnerjev EU projekta TRACE v Ljubljani, marec 2007.

FIGURE 4:
Workshop of partners of EU project TRACE in Ljubljana, March 2007.

- projekt *COST D2 (New fluororous media and processes for cleaner and safer chemistry);*
 - bilateralni projekt v okviru znanstveno-tehnološkega sodelovanja med Republiko Slovenijo in Republiko Makedonijo v letih 2007 in 2008 z naslovom Razvoj novih kemometrijskih procedur in algoritmov za študij relacij med kemijsko strukturo in aktivnostjo spojin; nosilca: dr. Marjana Novič in dr. Igor Kuzmanovski;
 - bilateralni projekt v okviru znanstveno-raziskovalnega sodelovanja med Republiko Slovenijo in Združenimi državami Amerike v letih 2006 – 2007 z naslovom Avtomatična primerjava in ovrednotenje proteomičnih podatkov; nosilca: dr. Marjana Novič in dr. Sol Bobst.
- Project IBAAC (*An Integrated Biomimetic Approach to Asymmetric Catalysis*) (Contract No. MCRTN –CT-2003-505020);
 - Project CAESAR (*Computer-Assisted Evaluation of industrial chemical Substances According to Regulations*) (SSPI-022674);
 - Project *COST D2 (New fluororous media and processes for cleaner and safer chemistry);*
 - Bilateral projects in the frame of Scientific and technological cooperation between Slovenia and Macedonia for the period 2007 and 2008 entitled "*Development of New Chemometric Procedures and Algorithms for Quantitative Structure-Activity Relationships Studies*". Principal investigators: Dr. Marjana Novič and Dr. Igor Kuzmanovski;
 - Bilateral project in the framework of scientific between Slovenia and Unites States of America in the years 2006 – 2007, entitled "*Proteomics data for automatic comparison and evaluation*". Principal investigators: Dr. Marjana Novič and Dr. Sol Bobst.

POMEMBNEJŠI INŠTRUMENTI IN DRUGA OPREMA

- Računalniška učilnica s 30 sedeži in 16 osebnimi računalniki;
- DIONEX-DX500 ionski kromatograf z novim avtomatskim vzorčevalnikom.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Kot vsako leto smo tudi letos povabili na štirimesečni delovni obisk profesorja Milana Randića, uveljavljenega raziskovalca na področju teorije grafov. Več let je že zunanji sodelavec naše programske skupine. V letu 2007 smo tudi uspešno konkurirali na javnem razpisu za (so)financiranje uveljavljenih raziskovalcev iz tujine, tako da smo za obisk profesorja Randića dobili dodatna sredstva in na tej osnovi izpeljali daljši obisk (maj – september 2007). 27. septembra 2007 je postal dr. Milan Randić častni član Kemijskega inštituta. Na slovesnosti ob podelitvi naziva je bil v uvodnem govoru poudarjen neprecenljiv prispevek prof. Randića k promociji Kemijskega inštituta in slovenske znanosti na področju teorije grafov in njene uporabe v računalniški kemiji. V predavanju je profesor Randić predstavil nekaj najpomembnejših dosežkov

IMPORTANT INSTRUMENTS

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

EDUCATION AND IMPORTANT VISITS

As every year, Professor Milan Randić, a recognized researcher in the field of graph theory, was invited for a 4-months research visit to our group. For several years he is an external collaborator of our research program P1-017. In 2007 we successfully applied at the national research agency ARRS for funding of his visit as an eminent foreign researcher. On this basis Professor Randić was staying in Ljubljana from May to September 2007.

On September 27th Professor Milan Randić became an honorary member of the National Institute of Chemistry. At the inauguration it has been stressed in the introductory speech how

zadnjih let in pokazal, kako s svežimi idejami sledi razvoju sodobne znanosti, tako da njegove najnovejše raziskave povezujejo matematično kemijo z novimi spoznanji na področju genomike in proteomike.

Naslednji raziskovalci iz tujine so vsaj en mesec, nekateri tudi celo leto, delali v našem laboratoriju:

- dr. Igor Kuzmanovski je poleg dokončanja projekta v okviru IBAAC raziskav (optimiranje dendrimerov, 7 mesecev) dopolnil svoje bivanje v našem laboratoriju z dodatnima dvema mesecema, v katerih je pripravil gradivo za objavo rezultatov, ki temeljijo na novo razviti metodi za optimiranje faktorjev vpliva posameznih spremenljivk v napovednih modelih inhibicije HIV-1 proteaze;
- dr. Sylwester Mazurek je v zadnjem mesecu bivanja kot IBAAC po-doktorski štipendist pripravil rezultate optimiranja ligandov v asimetrični katalizi za objavo. Rokopis je bil sprejet v objavo v *Molecular Diversity*;
- dr. Jaroslaw Panek je nadaljeval delo, ki ga je začel kot IBAAC štipendist. Poleg tega se je lotil zahtevne naloge določanja 3D strukture membranskega proteina bilitranslokaze, ki se je izkazalo za obetavno in ga bomo nadaljevali v prihodnjem letu.

Poleg tega smo na osnovi preteklega bilateralnega projekta z Indijo nadaljevali sodelovanje z dr. Manish-em Bagchi-jem, ki je dopolnil raziskave na modeliranju antituberkuloznih učinkovin. Literaturne podatke je vgradil v model, ki je ob poznavanju kemijske strukture sposoben napovedati antibakterijski učinek za spojine, ki so sorodne setu spojin uporabljenega podatkovnega niza.

Sodelavec Marjan Vračko je postal docent na Fakulteti za kmetijstvo Univerze v Mariboru za predmet Metode umetne inteligence v kmetijstvu. Tematika predmeta zaobsega modeliranje za ugotavljanje izvora hrane (tukaj smo pridobili precej izkušenj pri projektu TRACE), računalniško napovedovanje pridelka glede na naravne okoliščine in računalniško modeliranje toksičnosti biocidov.

important is his contribution for the promotion of the Institute and Slovenian science in the field of graph theory and its use in computational chemistry. During his lecture Professor Randić demonstrated some latest achievements and showed how he follows the trends in modern science with new ideas, so that he directed his recent research efforts into applications of graph theory to the field of genomics and proteomics.

The following researchers have spent at least one month, some of them a whole year, in our Laboratory:

- Dr. Igor Kuzmanovski completed the research within the IBAAC project (optimization of dendrimers, 7 months). He prolonged his stay for two months in the frame of the Slovenia-Macedonia bilateral project. During this time he prepared a publication of the results on the development of a new method for automatic adjustment of importance of variables in predictive models, designed for HIV-1 protease inhibitors.
- During the last month of his stay as IBAAC post-doctoral fellow Dr. Sylwester Mazurek prepared for publication the results on the optimization of ligands in asymmetric catalysis. The manuscript was accepted for publication in *Molecular Diversity*.
- Dr. Jaroslaw Panek continued his work on IBAAC project, which he has started as a post-doc fellow. Besides he started a new research work on the computational determination of a 3D structure of membrane protein bilitranslocase, which has turned out as a difficult but promising task and will be continued in the next year.
- In the framework of past bilateral cooperation with India we continued the collaboration with Dr. Manish Bagchi, who had accomplished the research on the modelling of antituberculosis drugs. The literature data were incorporated into a model, which is capable of prediction of antituberculosis effects for chemicals similar to those from the training set.

Sodelujemo tudi v dodiplomskem in podiplomskem študijskem programu kemometrije Fakultete za kemijo in kemijsko tehnologijo (FKKT) Univerze v Ljubljani: »Kemometrija v analizi kemiji«; na podiplomskem študiju s predmetom podobne vsebine v podiplomskem študiju kemije na FKKT Univerze v Ljubljani in podiplomskem študiju okoljske kemije na Fakulteti za gradbeništvo Univerze v Ljubljani. V lanskem letu smo bili sodelavci L03 mentorji ali komentorji petim doktorandom (dva tuja sta končala študij z zagovorom na Univerzi Milano Bicocca, Italija). Trije doktorandi opravljajo svoje doktorske raziskave v L03. Pomembno je tudi delovno mentorstvo pri diplomah, kjer smo sodelovali s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani: v letu 2007 je diplomiral Darko Butara, ki je imel delovnega mentorja v Laboratoriju za kemometrijo.

Dr. Marjan Vračko was promoted to a docent at Faculty of Agriculture of University of Maribor, Slovenia for the lessons on "Methods of artificial intelligence in agriculture". The subject encompasses modelling applied for origin of food (the benefit of our experience with TRACE EU project), for computerized prediction of crops regarding the natural conditions, and computational modelling of toxic biocides.

We contribute to the undergraduate and postgraduate studies of chemometrics: Faculty of Chemistry and Chemical Technology (FCCT), University of Ljubljana, »Chemometrics in analytical chemistry« and with a similar subject at postgraduate studies at the same faculty; and to the postgraduate studies of environmental chemistry at Faculty of Civil and Geodetic Engineering, University of Ljubljana.

In 2007 the coworkers of L03 provided mentorship to five PhD students. Two foreign students finished their studies in Italy, University Milano Bicocca, while three of them are young investigators in our Laboratory. It is worth mentioning the co-mentorship with a diploma student Branko Butara, who finished his undergraduate studies at FCCT, University of Ljubljana.

L04

Laboratorij za analizno kemijo

Analytical Chemistry Laboratory



VODJA / HEAD

dr. Božidar Ogorevc

RAZISKOVALCI / RESEARCHERS

dr. Bojan Budič
dr. Johannes T. van Elteren
dr. Irena Grgič
dr. Samo Hočevar
doc. dr. Milko Novič
dr. Vid Simon Šelih (od julija / from july)
dr. Janja Turšič (dopolnilno delovno razmerje /
part time)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Marija Slavec
Lea Mauko
Mersida Janeva
Darja Kotnik
Petra Apat

TEHNIČNO OSEBJE / TECHNICAL STAFF

Nuša Verbič
Breda Novak
Lidija Živec (polovični delovni čas / part time)
Helena Radić, dipl. ing. kem. (do novembra /
to november)
Vesna Lenarčič

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

Michael Beeston
Marjana Žnidar (do februarja / to february)
Barbara Ferenčak (do marca / to march)
Sabina Matjašec (do februarja / to february)
Alenka Okršlar (od oktobra/ from october)
Suzana Boškovič (od oktobra / from october)



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 vrstnih elementov in spojin pri reševanju okoljskih, biomedicinskih, atmosferskih, industrijskih idr. problematik. Strokovna znanja in izkušnje članov Laboratorija za analizno kemijo so zelo široke in pokrivajo med drugim področja kot so: elektrokemija (mikro-elektrode in senzorji), sklopljene tehnike (npr. tekočinska kromatografija in laserska ablacija v povezavi z ICP-masno spektrometrijo), ionska kromatografija, kemijski procesi v atmosferski vodni fazi, vzorčevanje in karakterizacija atmosferskih aerosolov (po velikostnih frakcijah), ICP-atomska emisijska spektrometrija, priprava vzorcev (razklop v mikrovalovni peči in sekvenčna/selektivna ekstrakcija) in modeliranje (ekstrakcijskih in separacijskih procesov). V naše raziskovalno delo so vključeni tudi podiplomski študenti, podoktorski gostje in specializanti. Dejavnost Laboratorija zajema tudi pogodbeno delo in storitve za neposredne industrijske in druge partnerje, kar vključuje razvoj in izboljšave

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 emphasis on development and adaptation of methods and analysis of all kind of samples (environmental, industrial, biological) and deter-

metod ter analize vseh vrst vzorcev (okoljski, industrijski, biološki) in določevanje praktično vseh elementov periodnega sistema kot tudi nekaterih anorganskih in organskih ionov.

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

BIBLIOGRAFIJA

- 8 izvirnih znanstvenih člankov
- 14 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 5 elaboratov, predštudij, študij
- 1 doktorat

GLAVNI DOSEŽKI V LETU 2007

- Na našem oddelku smo razvili in kot prvi na svetu objavili tankoslojno antimonsko elektrodo (SbFE), kot učinkovit senzor za elektrokemijsko stripping analizo težkih kovin v sledovih. SbFE je bila pripravljena in-situ na površini elektrode iz steklastega ogljika in uporabljena v povezavi z anodno stripping voltametrijo ali stripping kronopotenciometrijo. Takšna elektroda je izkazovala mejo zaznave $0,7 \mu\text{g L}^{-1}$ za Cd(II) in $0,9 \mu\text{g L}^{-1}$ za Pb(II). Primerjava z običajno uporabljano tankoslojno živosrebrovo elektrodo in z nedavno vpeljano tankoslojno bizmutovo elektrodo je pokazala izredne zmogljivosti SbFE, predvsem v bolj kislih medijih ($\text{pH} \leq 2$), kar je lahko prednost pri elektrokemijski analizi težkih kovin v sledovih v kombinaciji z uporabo "ne-živosrebrih" elektrod.
- V sodelovanju z ameriškim partnerjem smo razvili senzorski sistem, kjer smo uporabili magnetno prilagodljive nano-žičke, nanešene na površino osnovne elektrode iz steklastega ogljika za "na-ukaz" (on-demand) zaščito površine elektrokemijskega (stripping voltametričnega) senzorja, proti površinski aktivnim snovem. Nano-žičke omogočajo izpostavitve elektrodne površine med samim potekom elektrokemijskih meritev, oziroma nastavitve senzorja v zaščiteni (pasivni) način med posameznimi zaporednimi meritvami (slika 1). Delovanje nano-žičk, ki so sestavljene

mination 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/index.php?id=184>

BIBLIOGRAPHY

- 8 Original Scientific Articles
- 14 Published Scientific Conference Contribution Abstracts
- 5 Treatises, Preliminary Studies, Studies
- 1 Doctoral Dissertation

IMPORTANT ACHIEVEMENTS IN 2007

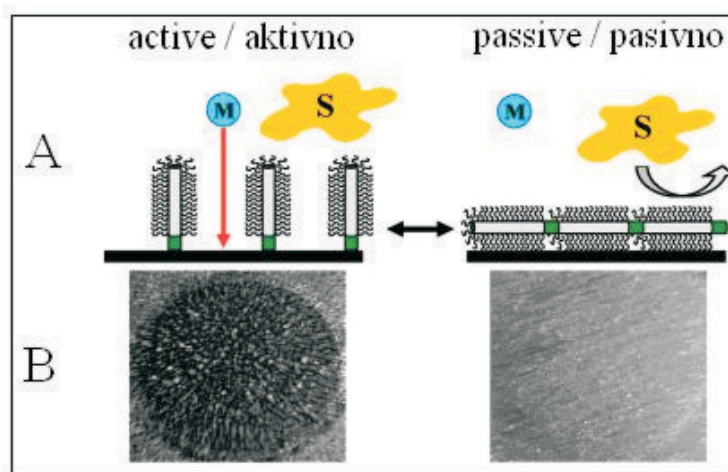
- For the first time an antimony film electrode (SbFE) developed in our Laboratory was demonstrated as a possible alternative for electrochemical stripping analysis of trace heavy metals. The SbFE was prepared in situ at a glassy carbon electrode and employed in combination with anodic stripping voltammetry or stripping chronopotentiometry. The SbFE exhibited a limit of detection of $0.7 \mu\text{g L}^{-1}$ for Cd(II) and $0.9 \mu\text{g L}^{-1}$ for Pb(II). Its comparison with the commonly used mercury film electrode and recently introduced bismuth film electrode revealed a remarkable performance, particularly in strong acidic solutions ($\text{pH} \leq 2$), what may be advantageous in the electrochemical analysis of trace heavy metals associated using a "mercury-free" electrode.
- In collaboration with our American partner the adaptive nano-wires deposited on the surface of a glassy carbon substrate electrode were used for the on-demand protection of an electrochemical (stripping voltametric) sensor against surface active compounds. The nano-wires offer periodic exposure of the electrode surface during the trace metal measurement step and setting the sensor in the protective (passive) mode between repetitive measurements (Figure 1) by switching magnetically the surface orientation of alkanethiol-coated gold nano-wires containing a short nickel (magnetic) segment be-

- iz zlatega dela, modificiranega z alkantiolom in iz kratkega magnetno-aktivnega nikljevega segmenta, je osnovano na magnetnem preklapljanju površinske orientacije nano-žičk med vertikalno (aktivno) in horizontalno (pasivno) orientacijo.
- Z uporabo laserske fotolize in absorpcije na dolgi optični poti (LFP-LPLA) smo določili konstante hitrosti za reakcije med SO_4^- radikalom in nekaterimi nizko-molekularnimi mono in dikarboksilnimi kisljinami in njihovimi anioni. Konstante za reakcije SO_4^- z glikolno, mlečno, jabolčno in malonsko kislino izmerjene v tej študiji so sploh prvič objavljene. Poleg tega smo z metodo inverznih hitrosti določili tudi reakcijske konstante za spiranje SO_4^- z vsemi omenjenimi organskimi kisljinami pri S(IV) oksidaciji katalizirani z Mn(II). Primerjava med temi konstantami in konstantami dobljenimi z direktnimi meritvami potrjuje predlagani inhibicijski mehanizem za S(IV) oksidacijo katalizirano z Mn(II) v prisotnosti monokarboksilnih kislin. Presentljivo pa dikarboksilne kisline kljub reaktivnosti z SO_4^- ne prispevajo k inhibiciji S(IV) oksidacije.
 - Z našim avstrijskim partnerjem smo sodelovali v sistematični študiji o ekstraktibilnosti arzenovih spojin iz certificiranega referenčnega materiala IAEA-140/TM (Fucus sp., homogenat morskih alg) z uporabo mešanic vode in metanola (od čiste vode do čistega metanola) z različnimi desorpcijskimi in topnostnimi lastnostmi in različnimi razmerji med volumnom ekstraktanta in maso vzorca (V/m). Razvili smo model na osnovi linearne sorpcijske izoterme, na osnovi katerega smo izračunali, da je bil maksimalni delež ekstraktabilnega arzena od 41 do 68% celokupne koncentracije arzena v CRM IAEA-140/TM, odvisno od sestave ekstraktanta. Glavne spojine v metanolno-vodnih ekstraktih so bili trije arzenosladkorji: glicerol riboza, sulfonat riboza in sulfat riboza, ki so skupaj predstavljali ca. 90% od maksimalno ekstraktabilnega arzena.
 - Between vertical (active) and horizontal (passive) positions.
 - The rate constants for reactions of the SO_4^- radical anion with some low molecular weight mono and dicarboxylic acids and their anions using the laser flash photolysis-long path laser absorption (LFP-LPLA) technique were determined. The present study contains the first measured rate constants for SO_4^- reactions with glycolic, lactic, malic and malonic acid. In addition, the rate constants for scavenging of SO_4^- by all investigated organics in the Mn(II)-catalyzed S(IV) autoxidation were determined by means of the reversed rate method. The comparison between these rate constants and the rate constants obtained by direct measurements confirms the proposed inhibiting mechanism for the Mn(II)-catalyzed S(IV) autoxidation in the presence of monocarboxylic acids. Surprisingly, although dicarboxylic acids are reactive towards SO_4^- they do not contribute to the inhibition of S(IV) oxidation.
 - Within the collaboration with our Austrian partner we took part in a systematic study on the extractability of arsenic species from algal certified reference material IAEA-140/TM (Fucus sp., Sea Plant Homogenate) using methanol/water extractant mixtures (from pure water to pure methanol), with different desorption and solubility parameters, and varying extractant volume to algal mass (V/m) ratios. A linear sorption isotherm-based model was developed to process the data showing that the maximal extractable arsenic fraction ranged from 41 to 68% of the total arsenic concentration in CRM IAEA-140/TM, depending on the extractant composition. The main arsenic species quantified in the methanol/water extracts were three arsenosugars: glycerol arsenosugar, sulfonate arsenosugar and sulfate arsenosugar, making up ca. 90% of the maximal extractable arsenic.
 - Collaborative work with our partner from Great Britain has led to the development of

- Sodelovanje z raziskovalci iz Velike Britanije je pripeljalo do razvoja novega analiznega postopka za merjenje mobilnosti elementov v prsti oz. tleh. Posebej v ta namen skonstruiran sistem omogoča, da v navpični koloni eluent obliva delce prsti, tako da so delci v neprestanem gibanju (fluidised bed princip). Eluent je nato iz navpične kolone speljan v masni spektrometer z induktivno sklopljeno plazmo (ICP-MS), s čimer lahko v realnem času spremljamo profile izluževanja elementov, ki kažejo na stopnjo vezanosti elementov v prsti (slika 2). Uporaba linearnega gradienta ekstraktanta od 0,05 mol l⁻¹ amonijevega sulfata do 0,11 mol l⁻¹ očetne kisline, omogoča vpogled v stopnjo vezanosti

an analytical tool for the determination of the elemental mobility in soil. Employing counter-current flow soil contacting in a fluidised bed (FB) column, in combination with on-line inductively coupled plasma mass spectrometry (ICP-MS), extraction profiles are produced which are representative for the behaviour of elements in soil (Fig. 2). Using a linear leachant gradient of 0.05 mol l⁻¹ ammonium sulphate to 0.11 mol l⁻¹ acetic acid, the associations present between the elements in the soil and their occurrence in multiple phases may be identified, hence giving an accurate assessment of the risk.

- A micro-electrode was developed based on a carbon paste comprising carbon nano-parti-



SLIKA 1:

Shematski in mikroskopski prikaz delovanja zaščitne senzorske površine z magnetno aktivnimi nano-žičkami.

A (levo): prikaz sheme nano-žičk na elektrodni površini postavljenih v vertikalni (aktivni) položaj; A (desno): nano-žičke postavljene v horizontalni (zaščiteni oz. pasivni) položaj.

B (levo): optična mikroskopska slika nano-žičk v vertikalnem (aktivnem) položaju; B (desno): v horizontalnem (pasivnem) položaju. Legenda: M - kovinski ion/analit, S - površinsko aktivna molekula.

FIGURE 1:

Schematic and microscopic image presentation of the sensor surface protection with magnetically-active nano-wires:

A (left): Scheme of nano-wires deposited on the electrode surface in vertical (active) position; A (right): Nano-wires in horizontal (passive) position.

B (left): Corresponding optical microscopic image of nano-wires in vertical (active) position. B (right): Nano-wires in horizontal (passive) position. Legend: M - metal ion/analyte; S- surface active compound.

elementov v prsti. Opazili smo različne profile izluževanja in prisotnost nekaterih elementov v več fazah, ti podatki pa omogočajo oceno tveganja kontaminantov v prsti.

- Razvili in skonstruirali smo mikro-elektrodo iz ogljikove paste, ki vsebuje ogljikove nanodelce s povprečnim premerom 30 nm in vezivno olje. Ogljikovo pasto smo vnesli v ohišja iz vlečenih steklenih kapilar s premeri od nekaj deset do manj kot deset mikrometrov ($r = 4.5 \text{ mm}$). Delovanje mikro-elektrode iz ogljikove paste je bilo omogočeno s pomočjo novo razvitega batnega sistema (slika 3). Karakteristike in uporabnost predlagane mikro-elektrode smo prikazali z elektrokemijskimi meritvami nekaterih potencialno zanimivih organskih in anorganskih analitov, kot so dopamin, askorbinska kislina in nekatere izbrane težke kovine.
- S pomočjo vrstične elektrokemijske mikroskopije (SECM) in mikroskopije na atomsko silo (AFM) smo preiskovali tankoslojne bizmutove elektrode, pripravljene ex-situ v prisotnosti ali odsotnosti bromidnih ionov v modifikacijski raztopini. Za študij prevodnosti in reaktivnosti tankih bizmutovih slojev, nanešenih na osnovno elektrodo iz steklastega ogljika, smo izbrali SECM povratni (feedback) način delovanja. Meritve so pokazale, da bromidni ioni, ki sicer povečajo stabilnost bizmutovih slojev, ne zmanjšajo bistveno njihove prevodnosti in reaktivnosti, AFM meritve pa so razkrile gostejšo rast manjših bizmutovih kristalov na površini osnovne elektrode v prisotnosti bromidnih ionov, medtem ko so bili v primeru njihove odsotnosti kristali večji in redkeje porazdeljeni.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V letu 2007 smo sodelovali z več deset industrijskimi in drugimi partnerji v okviru pogodb ali naročil za razvoj ali adaptacije in optimizacije metod oz. izdelave kemijskih analiz različnih vzorcev iz proizvodnje, okolja ali

cles with an average diameter of 30 nm and binding oil. The carbon paste was encased in pulled glass capillaries ranging in diameter from several tens down to less than ten micrometre ($r = 4.5 \text{ mm}$). Manipulation of the carbon paste micro-electrode was accomplished via a newly developed piston-driven system (Fig. 3). Characteristics and applicability of the proposed carbon paste micro-electrode was demonstrated by measuring some potentially interesting organic and inorganic analytes such as dopamine, ascorbic acid and selected heavy metals.

- Scanning electrochemical microscopy (SECM) and atomic force microscopy (AFM) were used to investigate the characteristics of bismuth film electrodes prepared ex-situ in the absence and presence of bromide ions in the modification solution. A SECM feedback mode was employed to examine the conductivity and reactivity of thin bismuth films deposited onto disk glassy carbon substrate electrodes. The measurements revealed that bromide ions, which enhance the stability of bismuth films, did not significantly compromise the conductivity and reactivity of bismuth films, whereas AFM measurements disclosed a denser growth of smaller bismuth crystals on the surface of substrate electrode in the presence of bromide ions, while the crystals were bigger but sparser in the absence of bromide ions.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

In 2007 we collaborated with several tens industrial and other partners within the framework of contracts, and other types of cooperation, for development and adaptation of methods and perform analyses of various samples from industrial processes, the environment and research, which require the analytical expertise and special instrumentation that the Analytical Chemistry Laboratory can provide owing to its research activity.

raziskav, ki zahtevajo posebna znanja in izkušnje ter specialno instrumentacijo, kar vse nudimo v našem laboratoriju. Med najpomembnejše industrijske partnerje tovrstnega sodelovanja v letu 2007 sodijo:

- Salonit Anhovo d.d., Deskle;
- Krka d.d., Novo mesto;
- Lek d.d., Ljubljana;
- Belinka Perkemija d.o.o., Ljubljana;
- Pivovarna Union d.d., Ljubljana;
- Melamin d.d., Kočevje;
- Regeneracija d.o.o., Lesce;
- Kolektor PRO d.o.o., Idrija;
- Tanin Sevnica;
- Zlatarna Celje d.d., Celje idr.

Sodelovanje z neindustrijskimi partnerji v letu 2007 je zajemalo pogodbeno in drugo razvojno in raziskovalno delo z naslednjimi neposrednimi partnerji:

- Agencija Republike Slovenije za okolje, Ljubljana;
- Elektroinštitut Milan Vidmar, Ljubljana;
- Ministrstvo za okolje in prostor, Ljubljana;
- Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani;
- Enota za patologijo prehrane in higieno okolja, NVI, Veterinarska fakulteta, Univerza v Ljubljani;
- Inštitut Jožef Stefan, Ljubljana;
- Fakulteta za strojništvo, Univerza v Mariboru;
- Zavod za gradbeništvo Slovenije, Ljubljana;
- Inštitut za hmeljarstvo in pivovarstvo Slovenije, Žalec;
- Laboratorij za astrofiziko osnovnih delcev in Laboratorij za raziskave v okolju, Univerza v Novi Gorici;
- Očesna klinika, Klinični center, Ljubljana;
- Laboratorij za raziskavo možganov, Inštitut za patološko fiziologijo, Medicinska fakulteta, Univerza v Ljubljani idr.

V letu 2007 smo nadaljevali z izvajanjem

A selected list of the most important slovene industrial partners in 2007 comprises:

- Salonit Anhovo d.d., Deskle;
- Krka d.d., Novo mesto;
- Lek d.d., Ljubljana;
- Belinka Perkemija d.o.o., Ljubljana;
- Pivovarna Union d.d., Ljubljana;
- Melamin d.d., Kočevje;
- Regeneracija d.o.o., Lesce;
- Kolektor PRO d.o.o., Idrija;
- Tanin Sevnica;
- Zlatarna Celje d.d., Celje ...

Non-industrial partners for contract and research and development work in 2007 comprises:

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

In 2007 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 and the Thermopower plant Šoštanj, Slovenia.

INTERNATIONAL COLLABORATION

In 2007 the Analytical Chemistry Laboratory team members were involved in the following

raziskovalno-aplikativnega projekta z naslovom "Vpliv emisijskih virov na onesnaženje zraka s trdnimi delci" v sodelovanju z Elektroinštitutom "Milan Vidmar" in Termoelektrarno Šoštanj.

MEDNARODNO SODELOVANJE

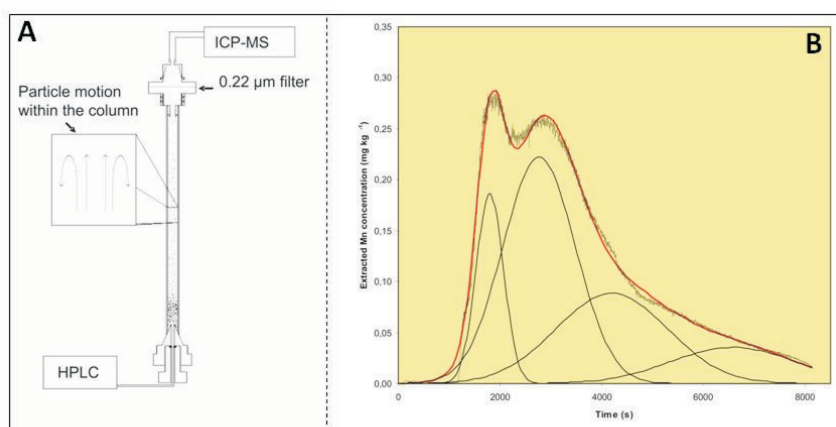
V letu 2007 so bili sodelavci Laboratorija za analizo kemijo vključeni v naslednje mednarodne projekte:

- INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change"). Raziskovalni mrežni program evropske znanstvene fundacije; trajanje: 2004-2008; nacionalna koordinatorica in članica vodstvenega odbora: I. Grgič.
- COST Action 633 "Particulate Matter: Properties Related to Health Effects", projekt poteka v okviru Evropske znanstvene fundacije; trajanje: 2002-2007; nacionalna koordinatorica ter podpredsednica COST 633: J. Turšič.
- Bilateralni projekt z naslovom "Razvoj novih elektrokemijskih (mikro) senzorjev z uporabo sodobnih materialov za meritve v biomedicini in okoljevarstvu" (BI-US/06-07/22) v okviru slovensko – ameriškega znanstvenega sodelovanja; trajanje 2006-2007; partner: prof. Joseph Wang, Arizona State University. Nosilec: S. Hočevar.
- Bilateralni projekt z naslovom "Uporaba laserske ablacije – induktivno sklopljene plazme masne spektrometrije za razumevanje antičnih/zgodovinskih tehnologij za izdelavo stekla in keramike" (BI-GB/07-013) v okviru slovensko – britanskega in Severno Irskega znanstvenega sodelovanja; partner: prof. Norman H. Tennent, Fyne Conservation Services, St. Catherine's, Scotland, UK. Nosilec: J. T. van Elteren.
- Bilateralni projekt z naslovom "Modeliranje separacijskih mehanizmov v moderni ionski kromatografiji: Določanje sledov anionov in kationov v kompleksnih vzorcih ter novi načini pred priprave vzorcev" (BI SLO-USA 07-07/ international projects:
 - A European Science Foundation Research Networking Programme INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change"); duration: 2004 - 2008; national coordinator and member of the Steering Committee: I. Grgič.
 - COST Action 633 project entitled "Particulate Matter: Properties Related to Health Effects" in the frame of European Science Foundation; duration: 2002 - 2007; national representative and vice-chair of COST 633: J. Turšič.
 - A bilateral project entitled "Development of novel electrochemical (micro)sensors using advanced materials for biomedical and environmental measurements" in the framework of S&T cooperation between Slovenia and USA 2006 – 2007. Partner: Prof. Joseph Wang, Arizona State University, USA. P.I.: S. Hočevar.
 - A bilateral project entitled "Exploration of the scope of laser ablation – inductively coupled plasma analysis in the field of conservation-restoration of cultural heritage comprising glass and ceramics" in the framework of S&T cooperation between Slovenia and Great Britain. Partner: Prof. Norman H. Tennent, Fyne Conservation services, St. Catherine's, Scotland, GB. P.I.: J. T. van Elteren.
 - A bilateral project entitled "Modelling of separation mechanisms in modern ion chromatography: The determination of traces of anions and cations in complicated matrices and new sample preparation tools and methods" in the framework of S&T cooperation between Slovenia and USA. Partner: PhD Christopher Pohl, Dionex Corporation. P.I.: Mi. Novič.
 - A bilateral project entitled "Formation and applications of Nanocomposite SOL-GEL thin films"; duration: 2007 - 2008. Partner: Prof. Daniel Mandler, The Hebrew University of Jerusalem. P.I.: B. Ogorevc.
 - A bilateral project entitled "Novel Approaches for Advanced Electrochemical Sensing" in the

- 29); partner: dr. Cristopher Pohl, Dionex Corporation. Nosilec: Mi. Novič.
- Bilateralni projekt med RS in Državo Izrael št. 1000-07-380012 z naslovom: "Priprava in uporaba nanokompozitnih SOL-GEL tehnik filmov"; trajanje: 2007-2008; partner prof. Daniel Mandler, The Hebrew University of Jerusalem. Nosilec: B. Ogorevc.
 - Bilateralni projekt z naslovom »Novi pristopi za sodobno elektrokemijsko detekcijo« (BI-CZ/07-08-008); partner: prof. dr. Karel Vytras, Univerza v Pardubicah, Pardubice, Češka. Nosilec: B. Ogorevc.
 - Sodelovanje v projektu z naslovom »Karakterizacija na nanometrijski skali« v okviru Centra odličnosti »Nanoznanosti in nanotehnologije«. Projekt je sofinanciran iz Evropskega sklada za regionalni razvoj.
- framework of S&T cooperation between the Republic of Slovenia and the Czech Republic; duration 2007 - 2008. Partner: prof. dr. Karel Vytras, University of Pardubice, Pardubice. P.I.: B. Ogorevc.
- Collaboration in a Project entitled "Characterization at Nanometre Scalq" in the frame of Center of Excellence "Nanosciences and Nanotechnologies". Project co-funded by the European Structural Fund, duration 2004 - 2007.

MAJOR EQUIPMENT

- Inductively coupled plasma mass spectrometer (ICP-MS, Agilent Technologies, Model 7500 ce&cs with additional accessories)
- Instrument for laser ablation (New Wave Research, Model UP 213 A/F)
- Inductively coupled plasma mass spectrometer (ICP-MS, Hewlett Packard, Model HP



SLIKA 2:

Prikaz delovanja posebnega analznega sistema za kontinuirano izluževanje elementov iz vzorcev prsti oziroma tal.

A: izluževanje kovin iz prsti z uporabo "fluidised bed" principa z ICP-MS detekcijo za vpogled v mobilnost kovin v prsti; B: profil izluževanja mangana (Mn), kjer dekonvolucija pokaže prisotnost več različnih faz.

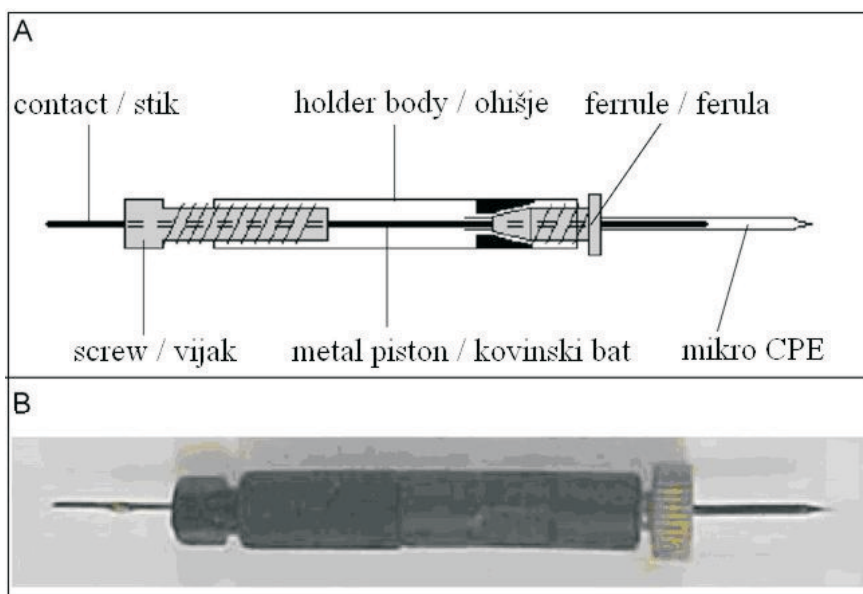
FIGURE 2:

Presentation of a special analytical tool for continuous extractions of elements from soil samples.

A: Diagram of the fluidised bed setup for gradient leaching of metals from soil with on line ICP-MS detection to unravel the mobility of metals in soil. B: Manganese (Mn) leaching profile where multiple phases have been quantified by deconvolution.

POMEMBNI INŠTRUMENTI IN OPREMA

- Masni spektrometer z induktivno sklopljeno plazmo (ICP-MS, Agilent Technologies, model 7500 ce&cs z dodatno opremo;
- instrument za lasersko ablacijo, New Wave Research, model UP 213 A/F;
- masni spektrometer z induktivno sklopljeno plazmo (ICP-MS, Hewlett Packard, model HP 4500 PLUS) s HPLC modulom in UV/Vis spektrometrom (DAD, Agilent, 1100 Series);
- atomski emisijski spektrometer z induktivno sklopljeno plazmo (ICP-AES, Thermo Jarrell Ash, Model Atomscan 25) opremljen z ultrazvočnim razpršilcem (Cetac, model U-6000 AT);
- vrstični elektronski mikroskop z visoko ločljivostjo (SEM) (Carl Zeiss, model SUPRA 35 VP) opremljen z energijsko disperzijskim spektrometrom (EDX) (Oxford Instruments, model Inca 400/SEM/EDX je skupna oprema
- 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)
- High resolution scanning electron microscope (SEM) (Carl Zeiss, model SUPRA 35 VP), equipped with an energy dispersive X-ray Spectrometer (EDX) (Oxford Instruments, model Inca 400) /SEM/EDX is shared with some other institute's research units/
- UV/Vis spectrophotometer (Perkin Elmer, model Lambda 25)
- Ion chromatography (IC) system with conductivity and spectrophotometric detection
- Flow injection analyzer (ASIA Ismatec)
- Three computer assisted electrochemical workstations (Autolab, Eco Chemie) and a



SLIKA 3:

Mikro elektroda iz ogljikove paste narejene na osnovi nano-delcev iz črnega ogljika.

A: shematski prikaz ohišja mikro-elektrode iz ogljikove paste; (B) fotografija mikro-elektrode iz ogljikove paste.

FIGURE 3:

Carbon paste micro-electrode based on carbon black nano-particles.

A: Diagram showing the carbon paste micro-electrode assembly. (B) Corresponding optical image.

- več organizacijskih enot na inštitutu/;
- UV/Vis spektrofotometer (Perkin Elmer, model Lambda 25);
 - sistem za ionsko kromatografijo (IC) s konduktometrično in spektrofotometrično detekcijo;
 - pretočno injekcijski analizator (ASIA Ismatec);
 - tri računalniško vodene elektrokemijske delovne postaje (Autolab, Eco Chemie).in en prenosni elektrokemijski sistem (PalmSens);
 - invertni optični mikroskop (Eclipse, Nikon);
 - oprema za izdelavo mikroelektrod (aparati za vlečenje kapilar, stereo leča, aparati za brušenje mikroelektrod, računalniško vodeni mikromanipulatori idr.);
 - reakcijska komora za raziskovanje reaktivnosti aerosolskih delcev pod kontroliranimi pogoji;
 - oprema za vzorčevanje aerosolov z Bernerjevimi nizkotlačnimi 10-stopenjskim kaskadnimi impaktorji;
 - mikrovalovna peč za razklope (MLS 1200 MEGA, Milestone);
 - sistem za pripravo čiste in ultračiste vode (Millipore) z Elix in Milli-Q Gradient enotama;
 - mikro in analizne tehtnice (Sartorius) nameščene v specialno klimatizirani tehtalnici (kontrola temperature in vlage) opremljeni z ionizatorjem;

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Obiski v tujini:

- I. Grgić je bila na eno-mesečnem delovnem obisku na Université de Provence, Laboratoire de Chimie et Environnement, Marseille, Francija. Obisk je bil financiran z ESF- Exchange Grant v okviru INTROP mrežnega programa. Naslov projekta: »In-Cloud Evaporation-Condensation Cycles as a Possible Source of Secondary Organic Aerosols (SOA)«;
 - S. Hočevar je bil na dvotedenskem obisku na Oddeleku za analizno kemijo Univerze v Pardubicah, Češka Republika v okviru portable electrochemical system (PalmSens)
- Inverted optical microscope (Eclipse, Nikon)
 - Microelectrode fabrication tools (capillary puller, stereo-zoom microscope, microelectrode beveler, computerised micromanipulator, etc.)
 - 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)
 - Micro and analytical balances (Sartorius) placed in a specialised air conditioned (temperature and humidity control) room equipped with an ion emitter
 - Water purification system (Millipore) including Elix and Milli-Q Gradient units

EDUCATION AND IMPORTANT VISITS

Visits abroad:

- I. Grgić, one month research visit, Université de Provence, Laboratoire de Chimie et Environnement, Marseille, France; Visit was financed by an ESF- Exchange Grant in the frame of INTROP Networking Programme. Project title: »In-Cloud Evaporation-Condensation Cycles as a Possible Source of Secondary Organic Aerosols (SOA)«.
- S. Hočevar, two-weeks research visit, Department of Analytical Chemistry, The University of Pardubice, Czech Republic in the frame of bilateral project of bilateral Project between Republic of Slovenia and Czech Republic entitled "Novel Approaches for Advanced Electrochemical Sensing".
- M. Slavec, six-weeks research visit, Department of Analytical Chemistry, The University of Pardubice, Czech Republic in the frame of bilateral project of scientific- technological collaboration between Republic of Slovenia and Czech Republic entitled "Novel Approaches for Advanced Electrochemical Sensing".

bilateralnega projekta z naslovom "Novi pristopi za sodobno elektrokemijsko detekcijo";

- M. Slavec je bil na šest-tedenskem obisku na Oddeleku za analizno kemijo Univerze v Pardubicah, Češka Republika v okviru bilateralnega projekta z naslovom "Novi pristopi za sodobno elektrokemijsko detekcijo";
- J. T. van Elteren in M. Janeva sta opravila enotedenski delovni obisk pri prof. A.C. Cefalasu na National Hellenic Research Foundation, Atene, Grčija na temo pulzne laserske depozicije.

Obiski iz tujine:

- Doc. S. Gligorovski iz Université de Provence, Laboratoire de Chimie et Environnement, Marseille, Francija je bil na eno-mesečnem delovnem obisku, ki je bil financiran z ESF-Exchange Grant v okviru INTROP mrežnega programa. Naslov projekta: »Size segregated chemical composition of atmospheric aerosol particles«;
- Michael Beeston je v letu 2007 pod vodstvom somentorja dr. van Elterena pri nas opravljal raziskovalno delo za izdelavo doktorske disertacije, ki jo je uspešno zagovarjal dne 17. 12. 2007 na University of Exeter (Velika Britanija);
- Lucia Baldrianova in Eva Tesarova iz Univerze v Pardubicah, Češka Republika sta bili na enomesečnem delovnem obisku v okviru bilateralnega projekta med RS in Češko Republiko;
- prof. dr. Karel Vytras iz Univerze v Pardubicah je bil na dvotedenskem delovnem obisku v okviru slovensko-češkega bilateralnega projekta;
- prof. dr. Joseph Wang iz Arizona State University, ZDA je bil na nekajdnevem obisku, med katerim mu je bil svečano podeljen naziv častni član Kemijskega inštituta.

ing".

- J. T. van Elteren and M. Janeve one-week work visit to Professor A.C. Cefalas at the National Hellenic Research Foundation, Athens, Greece on the topic of Pulsed laser deposition.

Visits from abroad:

- Assis. Prof. S. Gligorovski from Université de Provence, Laboratoire de Chimie et Environnement, Marseille, France, one month research visit. Visit was financed by an ESF-Exchange Grant in the frame of INTROP: Project title: »Size segregated chemical composition of atmospheric aerosol particles«.
- Michael Beeston has been on a year work visit under the supervision of his co-mentor, Dr. van Elteren from our laboratory. He successfully defended his Ph.D. Thesis on 17th December, 2007 at the University of Exeter, Great Britain.
- Lucia Baldrianova and Eva Tesarova from University of Pardubice, Pardubice, Czech Republic, one month research visit the frame of bilateral project between Republic of Slovenia and Czech Republic.
- Prof. Karel Vytras from University of Pardubice, Pardubice, Czech Republic: two week visit in the frame of bilateral project between Republic of Slovenia and Czech Republic.
- Prof. Joseph Wang from Arizona State University, USA: several day visit during which Prof. Wang was awarded "Honorary Member of the National Institute of Chemistry Slovenia.

L05

Laboratorij za kemijo,
biologijo in tehnologijo vod

Laboratory for Chemistry,
Biology and Technology of Water



VODJA / HEAD
prof. dr. Milenko Roš

RAZISKOVALCI / RESEARCHERS

doc. dr. Gregor D. Zupančič (namestnik vodje /
deputy head)
doc. dr. Andreja Drolc
doc. dr. Tatjana Tišler
dr. Magda Cotman
dr. Janez Vrtovšek
prof. dr. Jana Zagorc Končan

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Anita Jemec
Mag. Tanja Kurbus
Mirjana Bistan

TEHNIČNO OSEBJE / TECHNICAL STAFF

Jelka Jelnikar
Emil Meden
Matjaž Omerzel

PRIPRAVNIKI / TRAINEES

Carmen Gomez Ruiz (IAESTE)
Gregor Grom (2 mesečna študentska praksa / 2
months)
Petra Igljučar (3 mesečna študentska praksa / 3
months)



PODROČJA DEJAVNOSTI

- a) Raziskovalni program:
- Integralni pristop k preprečevanju onesnaževanja voda - (MVZT); nosilec: M. Roš.
- b) Raziskovalni in razvojni projekti:
- Aplikativni projekt »Razvoj sistemov za čiščenje odpadnih voda s kombinacijo bioloških šaržnih in membranskih procesov« (MVZT in HTZ I.P., Velenje); nosilec: Gregor D. Zupančič;
 - Razvoj postopka za stabilizacijo, mineralizacijo in higienizacijo blata iz malih čistilnih naprav (MVZT, KP Velenje); nosilec: G. D. Zupančič;
 - Meroslovna sledljivost v kemiji – vloga referenčnih materialov in referenčnih merjenj (MVZT); nosilka: A. Drolc;
 - Organiziranje medlaboratorijskih primerjav za laboratorije, ki izvajajo monitoring odpadnih vod (MOP-ARSO); nosilka: M. Cotman;
 - Zagotavljanje sledljivosti (Urad RS za meroslovje, MIRS); nosilka: A. Drolc;
 - Neradiološki monitoring reke Save (Nuklearna elektrarna Krško); nosilka: M. Cotman;

RESEARCH ACTIVITIES

- a) Research programme:
- Integrated Approach to Water Pollution Prevention (Ministry of Higher Education, Science and Technology, Republic of Slovenia) – Principal investigator: M. Roš.
- b) Research and applied projects:
- Development of Biological Wastewater Treatment Procedures Combining Sequencing Batch Process and Membrane Technology; (Ministry of Higher Education, Science and Technology, Republic of Slovenia, HTZ I.P. Velenje) – Principal investigator: G. D. Zupančič;
 - Procedure Development for Stabilization, Mineralization and Hygienization of Wastewater Sludge from Small WWTP; (Ministry of Higher Education, Science and Technology, Republic of Slovenia, Municipality of Velenje) – Principal investigator: G. D. Zupančič;
 - Metrological Traceability in Chemistry – Role of Reference Materials and Reference Measurements (Ministry of Higher Education, Science and Technology, Republic of

- Pridobivanje obnovljive energije iz organskih substratov (Pivovarna Union in Pivovarna Laško); nosilec: Gregor D. Zupančič;
 - Pridobivanje bioplina iz odpadkov IUV (Industrija usnja Vrhnika); nosilec: Gregor D. Zupančič;
 - Pridobivanje zelene energije iz odpadne vode in sosubstratov Karton Količevo (Inštitut za celulozo in papir); nosilec: Gregor D. Zupančič;
 - Proučevanje škodljivih učinkov in mehanizmov dolgotrajnega delovanja organofosfornih snovi na ljudi, živali in okolje in načrtovanje ustreznih protiukrepov; TP MIR06, vodja projekta: M. Harmel, Oikos, Domžale.
- c) Vzdrževanje sistema kakovosti v skladu s standardom SIST EN ISO/IEC 17025.

BIBLIOGRAFIJA

- 9 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 2 strokovna članka
- 2 samostojna znanstvena sestavka v monografiji
- 1 intervju
- 2 drugo učno gradivo
- 2 objavljena znanstvena prispevka na konferencah (vabljeni predavanja)
- 9 objavljenih znanstvenih prispevkov na konferencah
- 2 objavljena strokovna prispevka na konferencah
- 9 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 objavljeni povzete strokovnega prispevka na konferenci
- 1 patentna prijava
- 3 prispevki na konferencah brez natisa
- 3 vabljeni predavanja na konferencah brez natisa
- 8 končnih poročil o rezultatih raziskav
- 4 elaborati, predštudije, študije
- 2 izvedenski mnenji, arbitražni odločbi
- Expertises, Arbitration Decisions

- Slovenia) – Principal investigator: A. Drolc;
- Organization of Interlaboratory Comparisons for Slovenian Laboratories which Perform Monitoring of Waste Water (Environmental Agency of Republic of Slovenia) - Principal investigator: M. Cotman;
- Assuring traceability of results of measurements in area of waste water (MIRS-Metrological Institute of Republic of Slovenia) - Principal investigator: A. Drolc;
- Non-Radiological Monitoring of the Sava River (Nuclear Power Plant, Krško, Slovenia) - Principal investigator: M. Cotman;
- Renewable Energy Production from Organic Substrates; (Brewery Union and Brewery Laško, Slovenia); Principal investigator: Gregor D. Zupančič;
- Biogas Production from Tannery Waste (IU V Vrhnika, Slovenia); Principal investigator: Gregor D. Zupančič;
- Renewable »Green« Energy from Pulp and Paper Industry Wastewater and Various Co-Substrates; (Pulp and Paper Institute); Principal investigator: Gregor D. Zupančič;
- Study of Harmful Effects of Long Term Exposures of Organophosphorus Compounds to Human, Animals and Environmental and Plans for Corresponding Preventive Measures. TP MIR06. Principal researcher: M. Harmel, Oikos, Domžale, Slovenia.

c) Operation of laboratory according to requirements of the standard SIST EN ISO/IEC 17025.

BIBLIOGRAPHY

- 9 Original Scientific Articles
- 1 Review Article
- 2 Professional Articles
- 2 Independent Scientific Component Parts in a Monograph
- 1 Interview
- 2 Other Educational Material
- 2 Published Scientific Conference Contributions (Invited Lectures)
- 9 Published Scientific Conference Contributions

- 2 diplomi
- 1 magisterij
- 1 doktorat
- 2 uredništvi revij

GLAVNI DOSEŽKI V LETU 2007

- Preučevali smo kinetiko procesov biološkega čiščenja v dveh šaržnih reaktorjih pri visoki starosti oziroma koncentraciji biomase ($X > 10$ g/L). Prvi reaktor je deloval s klasično tehnologijo z dispergirano biomaso, v drugem pa smo uvajali novo tehnologijo čiščenja z granulirano biomaso. V obeh reaktorjih smo dosegli visoko učinkovitost čiščenja ob odličnih usedalnih lastnostih blata.
- Izvedli smo tudi prve preskuse na področju separacije mikroorganizmov z membranami (filtri). Kot filter smo uporabili material, katerega delovanje ne temelji na velikosti por, temveč na lastnostih nano delcev dodanega anorganskega materiala. Ti preskusi bodo služili kot osnova za študij na področju membranskih bioreaktorjev (MBR).
- Razvili smo aerobno tehnologijo obdelave blata za majhne čistilne naprave. Proces je prirejen za ČN do 5000 PE. Uporabili smo autotermalni efekt za doseglo higienizacije blata, pri tem smo pa precej povečali učinek odstranitve organskih komponent in hraniv, kot je amonijev dušik. Proces smo učinkovito testirali na napravi velikosti 150 PE.
- Razvili smo tehnologijo procesa za namen pridobivanja bioenergije - anaerobne obdelave polsuhih sipkih odpadnih organskih materialov, kjer smo rešili problem inhibicije procesa zaradi previsoke vsebnosti dušika v substratu.
- Razvili smo tehnologijo pridobivanja bioplina iz trdnih maščobnih odpadkov v kombinaciji z drugimi substrati brez predhodne termične obdelave maščob in s tem močno izboljšali toplotno bilanco procesa ter zmanjšali reaktorski volumen.
- Razvijali smo tehnologijo dodajanja odpadnih

- 2 Published Professional Conference Contributions
- 9 Published Scientific Conference Contribution Abstracts
- 1 Published Professional Conference Contribution Abstract
- 1 Patent Application
- 3 Unpublished Conference Contributions
- 3 Unpublished Invited Lectures at a Conference
- 8 Final Research Reports
- 4 Treatises, Preliminary Studies, Studies
- 2 Undergraduate Theses
- 1 Master's Thesis
- 1 Doctoral Dissertation
- 2 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2007

- Biological treatment processes were studied in two Sequencing Batch Reactors (SBRs). In the first SBR (anoxic/aerobic) high flocculent biomass concentration ($X > 10$ g/L) was achieved with long solid retention time (SRT). In the second SBR (aerobic) high biomass concentration ($X > 10$ g/L) was achieved with granulation. High treatment efficiency and good biomass settling properties were realised in both SBRs.
- Basic microfiltration tests with nano material membranes were performed for the introduction of the Membrane BioReactor (MBR) technology.
- We developed aerobic treatment of waste sludge from small WWTP's. The technology is suitable for WWTP's up to 5000 PE. We used auto-thermal properties achieve pathogen removal and at the same time managed to substantially increase volatile solids removal and nitrogen ammonia removal as well. The process was successfully tested in a device size of 150 PE.
- We developed the technology for anaerobic treatment of semisolid organic substrates for biogas production. We resolved the inhibi-

- so-substratov v anaerobni UASB sistem s ciljem povečanja proizvodnje bioplina brez povečanja reaktorskega volumna.
- Izvedli smo posebno medlaboratorijsko primerjavo »Nitrat v vodi«, namen katere je bilo ugotavljanje korelacij med uspešnostjo sodelovanja laboratorijev in različnimi faktorji (npr. uporabljena metoda merjenja, uveden sistem kakovosti, zagotavljanje sledljivosti, QA/QC,...).
 - Izvedli smo dve medlaboratorijski primerjavi za slovenske in tuje laboratorije, ki izvajajo monitoring odpadnih vod in delavnico na področju meroslovja v kemiji v sodelovanju z MIRS (Urad RS za meroslovje) in ARSO (Agencija Republike Slovenije za okolje).
 - Bili smo vpisani v mednarodno bazo EPTIS (BAM Nemčija), kot prva in edina slovenska shema medlaboratorijskih primerjav.
- tion problem of high nitrogen content in the substrate.
- We developed the technology for anaerobic treatment of solid fatty waste without thermal pretreatment. The heat balance of the process was improved as well as reactor volume reduced.
 - We have been developing the technology of addition of semi-solid substrates to anaerobic UASB reactor in order to increase biogas yield without increasing reactor volume.
 - Special Interlaboratory comparison »Nitrate in water« was organized in order to examine correlation between laboratories performance and influencing factors (ec. measurement method, implementation of quality system, traceability establishment, QA/QC,...).
 - We provided two distributions of samples in the ILC-Waste Water and organized work-



SLIKA 1:
Priprava vzorcev za Medlaboratorijske primerjave -
Odpadne vode 14 in 15 (2007)

FIGURE 1:
Sample preparation for Interlaboratory Comparison
– Waste Water 14 and 15 (2007)

- Vključili smo se v mednarodno mrežo organizatorjev medlaboratorijskih primerjav na področju vod v EU (v okviru projekta 6. OP EAQC-WISE).
- Študirali smo primernost biokemijskih biomarkerjev v vodnem raku kot nadgradnja obstoječih akutnih in kroničnih strupenostnih testov, ki temeljijo na ugotavljanju fizioloških odzivov. V vodnih bolhah smo spremljali aktivnost encimov po izpostavljenosti kovinam, pesticidom in različnim pripravkom pesticidov.
- Uvedli smo postopek za ugotavljanje normalnega razvoja zarodkov rib zebrič kot alternativno možnost obstoječega akutnega testa na preživetje rib za določanje strupenosti kemikalij in različnih voda.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

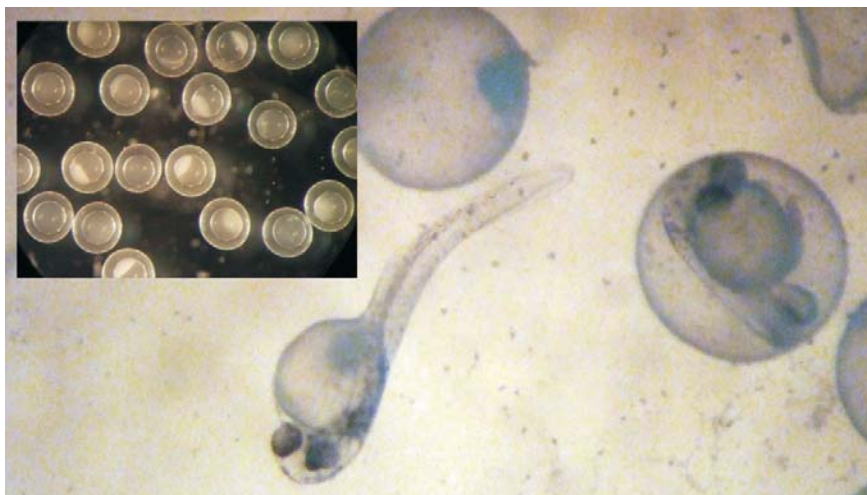
- Geološki zavod Slovenije, Ljubljana;
- Ministrstvo za okolje in prostor – Agencija RS za okolje, Ljubljana;
- Nuklearna elektrarna Krško, Krško;
- Univerza v Novi Gorici, Nova Gorica;

shop together with MIRS (Metrological Institute of Republic of Slovenia) and ARSO (Environmental Agency of Republic of Slovenia).

- The ILC-Waste Water is registered in the EPTIS database.
- We participated in »European Network of PTs providers supporting the implementation of the Water Framework Directive« (in the framework of the project 6. FP EAQC-WISE).
- The applicability of biochemical biomarkers in freshwater crustacean as an upgrade to conventional acute and chronic toxicity tests based on physiological responses was studied. The enzyme activities in water fleas were studied after the exposure to metals, pesticides and commercial products.
- A method based on development of fertilised zebrafish eggs was introduced as an alternative to existent acute toxicity test on zebrafish survival for toxicity evaluation of chemicals and different waters.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Geological Survey of Slovenia, Ljubljana, Slovenia;



SLIKA 2:
Razvoj zarodkov zebrič

FIGURE 2:
Development of zebrafish embryos

- Urad Republike Slovenije za meroslovje, Ljubljana;
- Zavod za gradbeništvo Slovenije (ZAG), Ljubljana;
- Pivovarna Laško, Laško;
- Pivovarna Union, Ljubljana;
- Industrija usnja Vrhnika, Vrhnika;
- Inštitut za celulozo in papir, Ljubljana;
- Komunalno podjetje Velenje, Velenje;
- Hidroinženiring, Ljubljana;
- Esotech d.d., Velenje;
- HTZ I.P., Velenje;
- Inštitut za raziskave v energetiki, ekologiji in tehnologiji, Ljubljana;
- Veterinarska fakulteta, Univerza v Ljubljani;
- Biotehniška fakulteta: Oddelek za biologijo in Oddelek za zootehniko, Univerza v Ljubljani;
- Biotehniška fakulteta: Oddelek za živilsko tehnologijo, Univerza v Ljubljani;
- Inštitut za fizikalno biologijo, Grosuplje;
- Oikos, Svetovanje za razvoj, Domžale;
- Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani.
- Ministry of Environment and Spatial planning – Environmental Agency of Republic of Slovenia;
- Nuclear Power Plant Krško, Krško, Slovenia;
- University of Nova Gorica, Faculty for Environmental Sciences, Nova Gorica, Slovenia;
- Metrology Institute of the Republic of Slovenia;
- Slovenian National Building and Civil Engineering Institute, Ljubljana, Slovenia;
- Laško Brewery, Laško, Slovenia;
- Union Brewery, Ljubljana, Slovenia;
- Tannery Industry Vrhnika, Vrhnika, Slovenia;
- Pulp and Paper Institute, Ljubljana, Slovenia;
- Municipality of Velenje, Velenje, Slovenia;
- Hidroinženiring, Ljubljana, Slovenia;
- Esotech d.d., Velenje, Slovenia;
- HTZ I.P., Velenje, Slovenia;
- Energy, Ecology and Technology Research Institute, Ljubljana, Slovenia;
- Veterinary faculty, University of Ljubljana, Slovenia;
- Biotechnical Faculty: Departments for Biology and Zootechnic, University of Ljubljana, Slovenia;

MEDNARODNO SODELOVANJE

- European Analytical Quality Control via Water Information System for Europe (EAQC-WISE), 6. OP, 2005-2008, pogodba št. 022603;
- European Network of PTs providers supporting the implementation of the Water Framework Directive;
- Training in Metrology in Chemistry (TrainMiC).
- Oikos, Development Consulting, Domžale, Slovenia;
- Institute of Physical Biology, Grosuplje, Slovenia;
- Biotechnical Faculty: Department for Food Technology, University of Ljubljana, Slovenia;
- Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia.

POMEMBNI INŠTRUMENTI IN OPREMA

- 5 Anaerobnih pilotnih reaktorjev z opremo;
- 2 Avtomatizirana šaržna biološka reaktorja (ŠBR);
- Anaerobni ŠBR reaktor;
- ATAD, polindustrijski šaržni reaktor;

INTERNATIONAL COLLABORATION

- European Analytical Quality Control via Water Information System for Europe (EAQC-WISE), 6. FP, 2005-2008, Contract no. 022603;
- European Network of PTs providers supporting the implementation of the Water Framework Directive;

- 2 UASB anaerobna reaktorja;
- Čitalec mikrotiterskih plošč (Bio-tek, Micro-Wave XS);
- Laboratorijski modeli bioloških čistilnih naprav;
- Laboratorijski modeli rek;
- Ionski kromatograf (DIONEX 120) s samodejnim vzorčevalnikom;
- Kjeltec sistem 2300 Autosystem II (FOSS Tecator) za razklop in določanje Kjeldahlovega dušika;
- Spektrofotometer Lambda 20 (Perkin-Elmer);
- TOC analizator TOC-5000A (SHIMADZU);
- LUMIS-TOX aparatura (dr. Lange);
- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector;
- Avtomatski KPK titrator Mettler-Toledo.

- Training in Metrology in Chemistry (TrainMiC).

MAJOR EQUIPMENT

- 5 Lab Scale anaerobic digesters with equipment;
- 2 Automated sequencing Batch Reactors (SBR);
- Anaerobic SBR reactor;
- ATAD-SBR reactor;
- 2 UASB reactors;
- Micro-plate reader (Bio-tek, Micro-Wave XS);
- Laboratory wastewater treatment plants;
- Laboratory river models;
- Ion chromatograph (DIONEX 120) with automated sampler (DIONEX);
- Kjeltec system 2300 Auto system II (FOSS Tecator) for Kjeldahl N determination;
- Spectrophotometer Lambda 20 (Perkin-Elmer);
- TOC analyser TOC-5000A (SHIMADZU);



SLIKA 3:
Anaerobni pilotni reaktorji

FIGURE 3:
Lab scale anaerobic digesters

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Izobraževanje:

- Doc. dr. Andreja Drolc je habilitirana na področju varstva okolja in predava predmet Onesnaževanje zraka, vode in tal (Univerza v Novi Gorici);
- Prof. dr. Milenko Roš je habilitiran za področje onesnaževanje in zaščita voda in predava predmet Zaščita voda (Univerza v Novi Gorici);
- Doc. dr. Tatjana Tišler je habilitirana za področje toksikologije in predava predmet Ekotoksikologija (Univerza v Novi Gorici);
- Doc. dr. Gregor D. Zupančič je habilitiran na področju varstva okolja (Univerza v Novi Gorici);
- Mentorstvo in somentorstvo ter delovno mentorstvo diplomskih, magistrskih in doktorskih del (M. Cotman, A. Drolc, M. Roš, T. Tišler, J. Vrtovšek, J. Zagorc-Končan, G. Zupančič).

Obiski in gostovanja:

- Soorganizacija delavnice »Primerljivost meritev v kemiji« (M. Roš, M. Cotman, A. Drolc);
- Soorganizacija konference z mednarodno udeležbo, VODNI DNEVI 2007, kjer so sodelavci laboratorija sodelovali kot predavatelji;
- Strokovna praksa v organizaciji IAESTE Ljubljana (Carmen Gomez Ruiz);
- Obisk inštituta Federal Research Centre for Fisheries, Institute for Fishery Ecology, Hamburg, Nemčija (A. Jemec, E. Meden).

- LUMIS-TOX apparatus (dr. Lange);
- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector;
- Mettler-Toledo automated COD titrator.

EDUCATION AND IMPORTANT VISITS

Education:

- Assist. Prof. Dr. Andreja Drolc is qualified as university teacher for the field *Environmental Protection*; she lectures the subject *Air, Water and Soil Pollution* (University of Nova Gorica, Slovenia);
- Prof. Dr. Milenko Roš is qualified as university teacher for the field *Water Pollution and Protection*; he lectures the subject *Water Protection* (University of Nova Gorica, Slovenia);
- Assist. Prof. Dr. Tatjana Tišler is qualified as university teacher for the field *Toxicology*; she lectures the subject *Ecotoxicology* (University of Nova Gorica, Slovenia);
- Assist. Prof. Dr. Gregor D. Zupančič is qualified as university teacher for the field *Environmental Protection*. (University of Nova Gorica, Slovenia);
- Mentorship at diploma, masters and doctoral theses (M. Cotman, A. Drolc, M. Roš, T. Tišler, J. Vrtovšek, J. Zagorc-Končan, G. Zupančič).

Important visits:

- Co-organisation of the workshop "Comparability of Chemical measurements" (M. Roš, M. Cotman, A. Drolc);
- Co-organisation of the conference with international participation, Water Days 2007, co-workers of the Laboratory were also lecturers;
- Technical practice for IAESTE Ljubljana (Carmen Gomez Ruiz);
- Working Visit of Federal Research Centre for Fisheries, Institute for Fishery Ecology, Hamburg, Germany (A. Jemec, E. Meden).

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
dr. Mitja Križman

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Maja Fir
Vesna Glavnik
Mitja Martelanc
Kajetan Trošt
Alen Albreht

TEHNIČNO OSEBJE / TECHNICAL STAFF

Mateja Puklavec

PRIPRAVNIKI / TRAINEES

Barbara Kapun
Petra Jazbec



PODROČJA DEJAVNOSTI

Raziskovalno in razvojno delo v Laboratorija za prehrabeno kemijo (L06) je usmerjeno predvsem na vrednotenje spojin naravnega izvora in razvoj ustreznih prehranskih dodatkov. Delo poteka v petih podskupinah na:

- razvoju novih prehrabnenih izdelkov in prehranskih dodatkov s funkcionalnimi lastnostmi;
- pripravi in vrednotenju specialne prehrane in prehrabneni 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 HACCP.

BIBLIOGRAFIJA

- 7 izvirmih znanstvenih člankov
- 1 intervju
- 2 objavljena znanstvena prispevka na

RESEARCH ACTIVITIES

Research and development activities are oriented into investigation of compounds from natural sources and development of food additives. Work is divided into five main fields:

- development of new food products and food additives with functional activities
- preparation and evaluation of special food and food engineering
- determination of compounds from natural sources by modern chromatographic and spectroscopic techniques
- development and validation of new analytical techniques and methods
- preventing of chemical risks considering good laboratory practice and good manufacturing practice (GLP and GMP), development and validation of analytical methods, technological validations, cleaning validations and HACCP.

BIBLIOGRAPHY

- 7 Original Scientific Articles
- 1 Interview
- 2 Published Scientific Conference Contributions

- konferencah
- 9 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 2 prispevka na konferencah brez natisa
- 1 elaborat, predštudija, študija
- 4 diplome
- 1 doktorat

- 9 Published Scientific Conference Contribution Abstracts
- 2 Unpublished Conference Contributions
- 1 Treatise, Preliminary Study, Study
- 4 Undergraduate Theses
- 1 Doctoral Dissertation

GLAVNI DOSEŽKI V LETU 2007

- V sodelovanju z zunanjimi raziskovalnimi institucijami in v sklopu lastnih projektov smo pripravili metode za vrednotenje in pripravo učinkovin, ki so pomembne za človekovo zdravje. Skupaj z Veterinarsko fakulteto smo razvili nove metode za kvantitativno vrednotenje sladkorjev v plazmi z masno spektrometrijo in s to metodo pri psih ugotavljali poškodovanost črevesne sluznice po zaužitju nekaterih zdravil. Razvili smo analizno metodo za določevanje vsebnosti CoQ10 v človeški plazmi in plazmi in tkivih raznih živali. Razvito metodo smo uporabili za vrednotenje biorazpoložljivosti vodotopnega CoQ10.
- V sodelovanju s Perutnino Ptuj d.d. smo izvedli študijo, s katero smo testirali možnost proizvodnje piščančjega mesa s povečano vsebnostjo CoQ10. Tako pridobljeno meso bo služilo pripravi funkcionalnih živil. Ugotavljali smo povezavo med koncentracijo CoQ10 v krvi in tkivih različnih piščančjih organov ter časom hranjenja teh piščancev z obogateno krmo. Rezultati so pokazali, da je v vseh tkivih prišlo do znatnega porasta koncentracije CoQ10 (tudi do 50%); piščanci hranjeni s CoQ10 so hitreje pridobivali na teži (približno 115%). V vseh tkivih je prišlo do rahlega znižanja vsebnosti holesterola. Frakcioniranje celice je pokazalo, da se je večina eksogenega CoQ10 akumulirala v celičnih membranah.
- Za vodotopno obliko koencima Q10, za katero smo v letu 2006 prejeli SI Patent 21783 in 21992 in na podlagi mednarodne prijave PCT Pat. Appl. PCT/SI2005/000013 (WO 2005/111224) pričeli v letu 2007 vlagati nacionalne prijave: RU Pat. Appl. 2006140641, EP Pat. Appl. 05738276.4, US

IMPORTANT ACHIEVEMENTS IN 2007

- In collaboration with partners from other research institutions and in the scope of our research projects, different analytical methods for evaluation of compounds important for human health were prepared.
- Together with Veterinary clinic we developed a new HPLC-MS method for quantitative evaluation of some sugars in blood. Method was successfully used for evaluation of damages produced by non-steroidal anti-inflammatory drug on permeability of dogs intestinal barrier. A new original analytical method for quantitative evaluation of CoQ10 in human plasma and different animal tissues was developed and used in bioavailability studies.
- In cooperation with Perutnina Ptuj d.d. we made the experiment in which we tested if it is possible to prepare chicken meat with increased amount of CoQ10. This meat will be used in functional food products. In all chicken tissues concentrations of CoQ10 increased considerably. Chickens fed with enriched fodder grow faster (nearly 115%). Accomplished study showed that major increase in concentration of CoQ10 in meat tissues up to 50%. In nearly all meat tissues concentration of cholesterol was slightly reduced. The fractionation of chicken breast tissue indicated that supplementary CoQ10 was primarily deposited in membranes.
- After we acquired two Slovenian patents SI Patent 21783 and 21992 in 2006 and on the base of international patent application PCT Pat. Appl. PCT/SI2005/000013 (WO 2005/111224) we started to apply our patent in selected countries; RU Pat. Appl.

- Pat. Appl. 11/569,110, IZ Pat. Appl., 179143.
- Izvedli smo »scale up« proizvodnjo vodotopnega Q10 na 30 litrskem računalniško vodenem reaktorju in sodelovali pri proizvodnji komercialnih količin.
 - Pripravili in ovrednotili smo funkcionalne prehrabene izdelke obogatene s CoQ10 (novi izdelki ali novi proizvajalci), med drugim mleko, jogurt, kefir, med, šumeče tablete, čokoladne izdelke in sokove. Izdelke smo kemijsko in organoleptično ovrednotili in jim določili stabilnost.
 - Z namenom priprave stabilnih sadnih sokov in njihove embalaže, smo v izbranih sokovih in koncentratih nadaljevali z določanjem vsebnosti skupnih polifenolov, skupnih antocianov, vitamina C in antioksidativne učinkovitosti. Identificirali in določili smo vsebnost posameznih antocianinov, flavonolov in fenolnih kislin. Preizkušali smo uporabnost embalaže s posebnimi antioksidativnimi lastnostmi in sinergistično delovanje specialne embalaže in antioksidativnih dodatkov. Spremembe smo ugotavljali z merjenjem kemijskih parametrov in s senzoričnimi določitvami.
 - Opravili smo več raziskav navadnega komarčka (*Foeniculum vulgare Mill.*). Razvili smo kvantitativno vrednotenje intragenomskega polimorfizma ribosomske DNA s PCR-RFLP markerji in odkrili 3 različne tipe zaporedij ITS regije. Opravili smo sočasno statistično vrednotenje kemijskega in molekulskega genetskega profila navadnega komarčka ter temu ustrezno prilagodili statistično metodo (Cavalli-Sforza in Edwards). Razvili smo tudi HPLC metodo (ob uporabi monolitne kolone) za določanje glavnih fenolnih spojin v navadnem komarčku.
 - Razvili smo analizo metodo za določanje likopena v prehranskem dopolnilu, kjer je bilo treba rešiti predvsem problem ekstrakcije nepolarnega in nestabilnega analita. Ker smo ugotovili, da je likopen prisoten v pre-
- 2006140641, EP Pat. Appl. 05738276.4, US Pat. Appl. 11/569,110, IZ Pat. Appl., 179143.
- The "scale up" pilot production on 30 L computer controlled reactor was done and we took an active part in production of commercial quantity of CoQ10.
 - Some new functional food products (milk, yogurt, kefir, chocolate and juices) with increased amount of CoQ10 were prepared and evaluated with chemical and organoleptic tests. Stability of the final products was also established.
 - In order to prepare stable form of fruit juices and packing material, special test samples were prepared and content and changes of concentrations of polyphenols, anthocyanins, vitamin C and antioxidant activity were measured. The influence of new packing materials with antioxidant properties and synergistic effect of these new material and antioxidants additives were tested. Differences were evaluated from acquired chemical and sensoric parameters.
 - We have conducted several research activities on fennel (*Foeniculum vulgare Mill.*). A quantitative procedure for polymorphism assessment of the ribosomal DNA region with PCR-RFLP markers developed and 3 different sequence types of the ITS region were found. A simultaneous statistical evaluation of fennel chemical and molecular genetic profile was done by means of an adapted statistical method (Cavalli-Sforza and Edwards). We also developed an HPLC method for the determination of phenolic compounds in fennel.
 - We developed an analytical method for determination of lycopene in dietary supplement. The main problem was the extraction of this nonpolar and unstable analyte. Since we found, that it was present in a complex with protein, we applied a novel approach using protease before its extraction into organic phase. We examined the form of the lycopene (»all«-*trans* or *cis* isomers, natural

hranskem dopolnilu v obliki kompleksa s proteinom, smo med drugim testirali tudi ekstrakcijo s pomočjo proteaze. Ekstrakcija je potekala tako, da smo v prvi fazi razgradili nosilni protein, nato pa ekstrahirali likopen v organsko fazo. Proučili smo obliko, v kateri je likopen prisoten (*cis* ali *all-trans* izomeri, sintetski ali naravni likopen) in ustreznost specifikacije na izdelku z dejansko vsebnostjo.

- Študirali smo vpliv saponifikacijskih pogojev (čas, temperatura, koncentracija baze itd) na lutein in estre luteina z višjimi maščobnimi kislinami, pri čemer so nam kot izvori teh spojin služila nekatera prehranska dopolnila in cvetovi žametnice. Vzorce žametnice smo pridobili v okviru bilateralnega projekta s Tobačnim inštitutom (Prilep), v katerem raziskujemo, če bi lahko žametnica vsaj deloma nadomestila tobačno kulturo v R. Makedoniji.
- Za določanje triterpenoidov in fitosterolov v različnih rastlinskih ekstraktih smo razvili nove kromatografske metode na osnovi tekočinske

or synthetic lycopene) and the suitability of the product label specification.

- We studied the influence of saponification conditions (time, temperature, concentration of base, etc) on lutein and lutein esters with high fatty-acids using some dietary supplements and Marigold (*Tagetes* species) flowers. The samples of *Tagetes* were obtained in the frame of bilateral project with Tobacco Institute (Prilep), in which we investigate the potential of *Tagetes* as an alternative crop on tobacco fields in Republic of Macedonia.
- New analytical methods based on high-performance liquid chromatography (HPLC-UV and HPLC-MS) and thin-layer chromatography for determination of triterpenoids and phytosterols in different plant extracts were developed. These methods were used within the cooperation with researchers from Biotechnical Faculty (Department of Agronomy, Ljubljana, Slovenia) in the investigation of differences in natural resistance of



SLIKA 1
HPLC-MS LCQ, Finnigan

FIGURE1
HPLC-MS LCQ, Finnigan

kromatografije visoke ločljivosti (HPLC-UV in HPLC-MS) in tankoplastne kromatografije. Te metode smo v sodelovanju z raziskovalci z Biotehniške fakultete (Oddelek za agromonomijo) uporabili za raziskave razlik v naravni odpornosti enaindvajsetih sort zelja proti izbranim insektom.

- Razvili in optimizirali smo detekcijski reagent za denzitometrično določanje katehinov v čokoladi ter študirali pogoje ekstrakcije katehinov iz različnih vzorcev, še posebej pa iz kakava in čokolade, kar smo izvedli v okviru bilateralnega projekta z raziskovalci s Fakultete za kemijsko inženirstvo in tehnologijo Univerze v Zagrebu, Hrvaška. Na osnovi tankoplastne kromatografije z denzitometrijo smo razvili in validirali analizo metodo za kvantitativno določanje epikatehina in procianidina B2 v kakavu in čokoladi.
- S skupino s Fakultete za farmacijo Univerze v Beogradu smo v okviru bilateralnega projekta razvili metodo za določanje 15 gvanidinskih/imidazolinskih derivatov (hipertenzivov). Gre za metodo na osnovi elektrokinetične kromatografije (EKC), ki je uporabna tudi za QSAR študije ter za proučevanje inkluzijskih kompleksov teh s spojin z β -ciklodekstrinom, ki se pogosto uporablja kot matriks v farmacevtskih formulacijah. Poleg tega smo razvili tudi dve metodi za določanje spojin (zdravil) iz skupine ACE inhibitorjev na HPTLC silikagelski in na monolitnih UTLC ("ultra thin-layer chromatographic") ploščah.
- Prilagodili smo obstoječo metodologijo za določanje vsebnosti aminokislin v vzorcih biološkega izvora, preko alkilfromil derivatov in separacije s plinsko kromatografijo. S tako prilagojeno GC metodo smo opravili študijo vrednotenja aminokislinske sestave gojišč humanih embrijev pri postopku umetne oploditve.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

Sodelovanje je potekalo s slovenskimi podjetji:
- Lek d.d., Ljubljana;

twenty-one different sorts of cabbage against the chosen harmful insects.

- We developed and optimised a detection reagent for densitometric determination of catechins in chocolate. Additionally, we studied conditions for extraction of catechins from different samples, especially from cocoa and chocolate, which was performed in the frame of bilateral project with Faculty of Chemical Engineering and Technology, University of Zagreb. We developed and validated a new thin-layer chromatographic method for determination of epicatechin and procyanidin B2 in cocoa and chocolate.
- In the frame of bilateral project with the group from University of Belgrade (Faculty of Pharmacy) we developed an electrokinetic chromatography (EKC) method for the separation of 15 guanidine/imidazoline derivatives acting as antihypertensive drugs. The method is also suitable for QSAR studies and studies of β -cyclodextrin inclusion complexes, since β -cyclodextrin is a common matrix used in pharmaceutical formulations. Two methods for determination of compounds from the group of ACE inhibitors using HPTLC silicagel and monolith UTLC ("ultra thin-layer chromatographic") plates were also developed.
- An existing methodology was adapted for the determination of amino acids from samples of biological origin, by means of alkylformyl derivatives and separation by GC. With the adapted GC method, a study for the determination of amino acid composition in human embryo culture media in the process of artificial fertilization was conducted.

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.,

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

in z institucijami:

- Klinični center, Ljubljana;
- Veterinarska fakulteta, Univerza v Ljubljani;
- Veterinarska klinika, Ljubljana;
- Zavod za zdravstveno varstvo Maribor;
- Biotehniška fakulteta, Univerza v Ljubljani;
- Inštitut za varovanje zdravja, Ljubljana;
- Nacionalni inštitut za biologijo, Ljubljana itd.

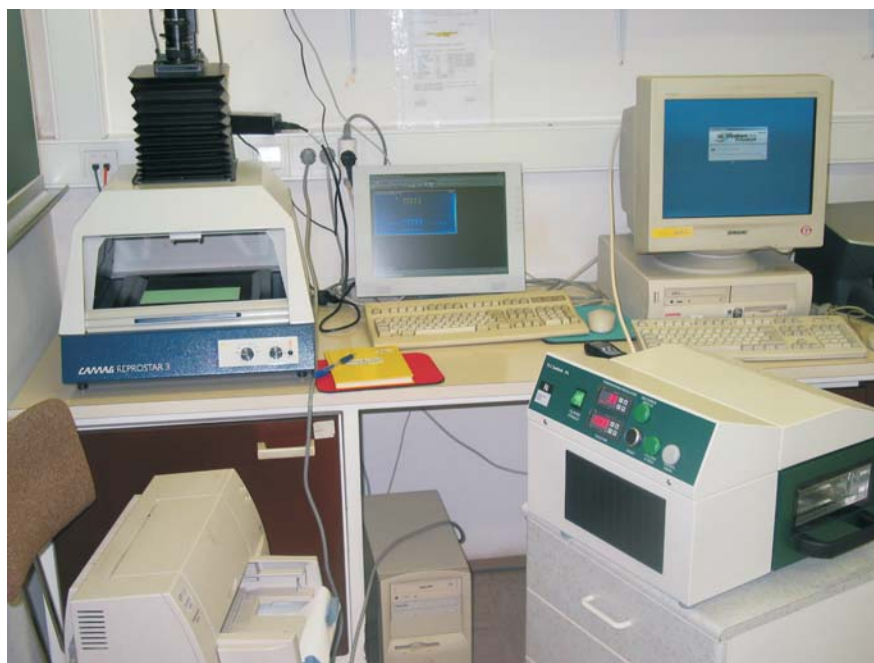
MEDNARODNO SODELOVANJE

- Evropski projekt: TEMPUS »Novi kurikularni modeli za izobraževanje prehrabnih

Ljubljana, Slovenia) and institutions (Medical Centre Ljubljana, Slovenia; Veterinary Faculty, University of Ljubljana, Slovenia; Veterinary clinic, Ljubljana, Slovenia; Biotechnical Faculty, University of Ljubljana, Slovenia; Institute for Public Health Maribor, Slovenia; National Institute of Biology, Ljubljana, Slovenia).

INTERNATIONAL COLLABORATION

- European project: »New curriculum models for educating food engineers« (TEMPUS CD_JEP-40065-2005), 2006-2009, principal researcher at NIC: B. Simonovska
- Bilateral project Slovenia - Croatia: »Development of chromatographic methods for determination of proanthocyanidins in food and nutraceuticals«, with University of Zagreb, Faculty of Chemical Engineering and Technology (Zagreb), principal researchers: I. Vovk and S. Babić



SLIKA 2

Testiranje naprave za kontrolirano sušenje kromatografskih plošč ("TLC sušilnik" razvit na Kemijskem inštitutu; SI patent št. 21199)

FIGURE 2

Testing of device for controlled drying of thin-layer chromatographic plates ("TLC Dryer" developed at the National Institute of Chemistry, SI patent No. 21199)

- tehnologov« (TEMPUS CD_JEP-40065-2005), 2006-2009, nosilka na KI: B. Simonovska;
- Bilateralni projekt Slovenija - Hrvaška s Fakulteto za kemijsko inženirstvo in tehnologijo Univerze v Zagrebu, Hrvaška: »Razvoj kromatografskih metod za določanje proantocianidinov v hrani in prehranskih dopolnilih«, nosilki: I. Vovk in S. Babić;
 - Bilateralni projekt Slovenija – Makedonija z University of St. Kliment Ohridski (Bitola), Tobacco Institute (Prilep): »Uvajanje novih rastlinskih kultur z biološko aktivnimi komponentami zanimivimi za prehrabeno in farmacevtsko industrijo«, nosilca: B. Simonovska in K. Filiposki;
 - Bilateralni projekt Slovenija - Srbija s Fakulteto za farmacijo Univerze v Beogradu: »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.

POMEMBNI INSTRUMENTI IN OPREMA

- HPLC sistemi z različnimi detektorji (UV/VIS, fluorescenčni in detektor z nizom diod);
- HPLC-MS sistema LCQ in TSQ, Finnigan;
- GC-17A s FID detektorjem, Shimadzu;
- GC-MS TRACEULTRA DSQ, Finnigan;
- vzorčevalnik iz parne faze (headspace do 210 °C) Perkin Elmer HS40XL (možnost priklopa na oba GC sistema);
- CE: Spectra Physics Spectra Phoresis 500 z UV-VIS detektorjem;
- Avtomatski vzorčevalnik: TLC automatic sampler 4, Camag;
- Sistemi za polavtomatsko nanašanje: Linomat IV in Linomat 5, Camag;
- Densitometer: TLC scanner 3, Camag;
- Sistem za video dokumentacijo in vrednotenje TLC kromatogramov: DigiStore 2 documentation system;
- SPE: Zymark Rapid Trace.

- Bilateral project: Slovenia – Macedonia: »Introduction of new crops with biologically active compounds interesting for the food and pharmaceutical industry« with University of St. Kliment Ohridski (Bitola), Tobacco Institute (Prilep); principal researchers: B. Simonovska and K. Filiposki
- Bilateral project: Slovenia – Serbia: "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

MAJOR EQUIPMENT

- HPLC systems with different detectors (UV/VIS, fluorescence and diode array)
- HPLC-MS systems LCQ in TSQ, Finnigan
- GC-17A with FID detector, Shimadzu
- GC-MS TRACEULTRA DSQ, Finnigan
- headspace sampler (up to 210 °C) Perkin Elmer HS40XL (connectable to both GC systems)
- CE: Spectra Physics Spectra Phoresis 500 with UV-VIS detector
- TLC automatic sampler 4, Camag
- TLC application systems: Linomat IV and Linomat 5, Camag
- Densitometer: TLC scanner 3, Camag
- System for video documentation and evaluation of TLC chromatograms: DigiStore 2 documentation system
- SPE Zymark Rapid Trace

EDUCATION AND IMPORTANT VISITS

In 2007 Mitja Križman defended Ph.D. dissertation. Four students from University of Ljubljana: Faculty of Chemistry and Chemical Technology (Luka Milivojević, Darja Groznik), Biotechnical Faculty (Ksenja David) and Faculty of Education (Katja Zavrl) finished their practical work in our Laboratory and took diplomas.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

V letu 2007 je Mitja Križman doktoriral. Štirje študenti s Fakultete za kemijo in kemijsko tehnologijo (Luka Milivojevič, Darja Groznik), Biotehniške fakultete (Ksenja David) in Pedagoške fakultete (Katja Zavrl) Univerze v Ljubljani so v Laboratoriju za prehrabeno kemijo opravili praktični del diplome in tudi diplomirali. Obiski:

- v okviru projekta TEMPUS: prof. dr. Slobodanka Kuzmanova, prof. dr. Eleonora Winkelhausen, prof. dr. Abdurauf Prusi, prof. dr. Aco Dimitrovski;
- v okviru bilateralnega projekta s Fakulteto za kemijsko inženirstvo in tehnologijo Univerze v Zagrebu, Hrvaška: doc. dr. Sandra Babić, dr. Dragana Mutavdžić Pavlović, dr. Danijela Ašperger;
- v okviru bilateralnega projekta s Tobacco Institute (Prilep, Makedonija), University of St. Kliment Ohridski (Bitola, Makedonija): dr. Marija Srbinoska;
- v okviru bilateralnega projekta s Fakulteto za farmacijo Univerze v Beogradu, Srbija: prof. dr. Danic Agbaba, prof. dr. Gordana Popović, Slavica Filipić (Ph.D. student).

Visits:

- In the frame of the European project TEMPUS: Prof. Dr. Slobodanka Kuzmanova, Prof. Dr. Eleonora Winkelhausen, Prof. Dr. Abdurauf Prusi, Prof. Dr. Aco Dimitrovski
- In the frame of bilateral project with Faculty of Chemical Engineering and Technology, University of Zagreb, Croatia: Dr. Sandra Babić, Assist. Prof., Dr. Dragana Mutavdžić Pavlović, Dr. Danijela Ašperger
- In the frame of bilateral project with Tobacco Institute (Prilep, Macedonia), University of St. Kliment Ohridski (Bitola, Macedonia): Dr. Marija Srbinoska
- In the frame of bilateral project with Faculty of Pharmacy University of Belgrade, Serbia: Prof. Dr. Danic Agbaba, Prof. Dr. Gordana Popović, Slavica Filipić (Ph.D. student)

L07

Laboratorij za polimerno
kemijo in tehnologijo

Laboratory for Polymer
Chemistry and Technology



VODJA / HEAD

izr. prof. dr. Majda Žigon

RAZISKOVALCI / RESEARCHERS

dr. Alojz Anžlovar
dr. Miroslav Huskić
mag. Edita Jasiukaityte
dr. Andrej Kržan
doc. dr. Matjaž Kunaver
dr. Ida Mav Golež
doc. dr. Ida Poljanšek (od / from 1. 3. 2007)
dr. Ema Žagar

**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Blaž Brulc
Maja Gričar
Tina Šmigovec
David Pahovnik (od / from 1. 10. 2007)

PRIPRAVNICA / TRAINEE

Jasmina Turnšek (od / from 26. 7. 2007)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Miran Lavrič
Polona Prosen
Meta Skumavc
Mirjana Širca



PODROČJA DEJAVNOSTI

Raziskave so potekale v okviru raziskovalnega programa P2-0145-0104 (Polimeri s posebnimi lastnostmi), temeljnih in aplikativnih projektov, projektov za industrijske partnerje, projekta 6. Okvirnega programa EU, evropske mreže odličnosti in bilateralnih projektov.

Področja dejavnosti L07 so:

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

RESEARCH ACTIVITIES

Research was conducted in the frame of the research programme P2-0145-0104 (Specialty Polymers), basic and applied projects, projects with industrial partners, European project (6th FP), Network of Excellence (6th FP), and bilateral research projects.

Research activities of L07:

- Biodegradable polymers
- Hyperbranched polymers
- Polymers from renewable resources
- Conductive polymers and composites
- Nanoparticles, polymer-based nanocomposites
- Self-cleaning photocatalytic coatings
- Coating systems with low VOC content
- Recycling of synthetic polymers
- Properties of polymers and polymeric materials
- Applied and development research, especially in the area of binders, thermoplastics, and recycling
- Analysis and characterization of research and commercial polymers by spectroscopic (FTIR, NMR), chromatographic (GC, GC-MS, IGC,

BIBLIOGRAFIJA

- 8 izvirnih znanstvenih člankov
- 1 strokovni članek
- 1 intervju
- 1 priročnik, slovar, leksikon, atlas, zemljevid
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanje)
- 6 objavljenih znanstvenih prispevkov na konferencah
- 30 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 3 patentne prijave
- 1 predavanje na tuji univerzi
- 2 prispevka na konferencah brez natisa
- 3 elaborati, predštudije, študije
- 1 izvedensko mnenje, arbitražna odločba
- 2 diplomi
- 8 uredništvev revij

GLAVNI DOSEŽKI V LETU 2007

- Organizacija Evropskega polimernega kongresa 2007 (European Polymer Congress 2007, 2. – 6. julij 2007, Portorož). Z več kot 800 udeleženci s celega sveta je bil kongres največji evropski dogodek na polimernem področju v letu 2007 in kot tak predstavlja največji dosežek laboratorija.
- Diblokkopolimere poli(L,L-laktid-*b*-β-benzil L-aspartat), PLBA, z definirano strukturo smo sintetizirali s polimerizacijo z odpiranjem obroča L,L-laktida na reaktivnih aaminskih skupinah poli(β-benzil L-aspartata) kot koincatorja in kositrovega(II) 2-etilheksanoata kot iniciatorja. Pri temperaturah nad 55°C je potekla delna hidroliza končnih benzilnih estrskih skupin, kar je vplivalo na nastanek delno razvejenih PLBA blok-kopolimerov. Vodotopne naključne kopolimere L-asparaginske kisline in L,L-laktida smo sintetizirali s polimerizacijo v talini.
- Raziskali smo vpliv staranja visoko razvejenega poliestra na osnovi 2,2-bis(metilol)propionske kisline druge psevdogeneracije (Boltorn® H20) v primerjavi s četrto psevdogeneracijo (Boltorn® H40) na preureditev mikrostrukture

SEC, SEC-MALS) and thermal techniques (DSC).

BIBLIOGRAPHY

- 8 Original Scientific Articles
- 1 Professional Article
- 1 Interview
- 1 Manual, Dictionary, Lexicon, Atlas, Map
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 6 Published Scientific Conference Contributions
- 30 Published Scientific Conference Contribution Abstracts
- 3 Patent Applications
- 1 Invited Lecture at Foreign University
- 2 Unpublished Conference Contributions
- 3 Treatises, Preliminary Studies, Studies
- 1 Expertise, Arbitration Decision
- 2 Undergraduate Theses
- 8 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2007

- Organization of the European Polymer Congress 2007 (July 2-6, 2007, Portorož, Slovenia). With over 800 participants from all over the world the congress represents the largest European event in the polymer area in 2007. The event undoubtedly represents the most significant achievement of the Laboratory.
- Diblock copolymers poly(L,L-lactide-*block*-β-benzyl L-aspartate), PLBA, with well defined structure were synthesized by ring opening polymerization of L,L-lactide using poly(β-benzyl L-aspartate) with amino end-groups as a coiniciator and tin octoate, SnOct₂, as an initiator. Partial hydrolysis of benzyl ester groups at the temperatures higher than 55°C led to partially branched PLBA copolymers. The random water soluble copolymers of L-aspartic acid and L,L-lactide were synthesized by polymerization in melt.
- We investigated the effects of annealing on the rearrangement of the H-bond network microstructure and its influence on the ther-

- in posledično na njune termične in reološke lastnosti.
- Zaključili smo delo na simulaciji delovanja mikrovalov na kemijsko reakcijo. Na primeru hidrolize enostavnega estra smo potrdili hipotezo, da vroča rotacijska stanja vodijo do povišane hitrosti reakcije.
 - Optimizirali smo proces utekočinjenja lesa z uporabo p-toluensulfonske kisline kot katalizatorja, pri čemer je bil izkoristek več kot 95 %. Iz utekočinjenega lesa in odpadnega papirja smo z adipinsko kislino sintetizirali linearni poliester za pripravo trdih poliuretanskih pen. Rezultati meritev natezne trdnosti pri 10% strižnih silah so pokazali, da imajo pene podobne lastnosti kot trde pene za izolacijo v gradbeništvu.
 - Razvili smo lepila na osnovi utekočinjenega lesa za različne namene. To lepilo ima bistvene prednosti pred analognimi komercialnimi lepili.
 - Potekajo preliminarne raziskave o uporabi utekočinjenega lesa kot alternativnega goriva. Specifična sežigna toplota je okrog 22MJ/kg, kar je mnogo več od rjavega premoga.
 - Pripravili smo prevodne filme z dobrimi mehanskimi lastnostmi iz mešanice dedopiranega polianilina (PANI) in njegovih derivatov s polimernimi dopanti: poliakrilno kislino, kopolimerom poli(asparaginska kislina-komlečna kislina) in anorgansko kislino $H_4SiW_{12}O_{40} \times 39 H_2O$.
 - Iz metil- in oktildietanolamina ter kislinskih kloridov smo sintetizirali različne poliestrske hidrokloride, s katerimi smo modificirali montmorillonit (MMT). Na debelino plasti MMT ni vplivala velikost kislinskega ostanka v poliesteru, pač pa dolžina alkilne stranske verige.
 - S poliolo metodo smo sintetizirali nanodelce in nanožičke ZnO velikosti 20 – 100 nm in pripravili nanokompozite s polimetilmetakrilatom, PMMA. Nanokompoziti PMMA/ZnO so transparentni, učinkovito absorbirajo UV mal and rheological properties of the second pseudo-generation hyperbranched polyester based on 2,2-bis(methylol)propionic acid (Boltorn® H20) in comparison to the fourth pseudo-generation HB polyester (Boltorn® H40).
 - We finished work on the simulation of the effects of microwaves on the chemical reaction. Using the example of ester hydrolysis we have confirmed our hypothesis that rotationally hot species lead to reaction acceleration.
 - We synthesized linear polyesters using liquefied wood as well as liquefied waste paper. Such polyesters were then used for the synthesis of rigid polyurethane foams with values for compressive strength at 10 % strain similar to those of standard foams, used for isolation purposes.
 - We developed novel adhesives based on liquefied wood for diverse applications. They have significant advantages in comparison to analogous commercial adhesives.
 - Preliminary research on utilizing liquefied wood as a liquid fuel has been conducted. The energy value is around 22MJ/kg, much more than that of brown coal.
 - Conductive films with good mechanical properties were prepared from the mixtures of dedoped polianiline or its derivatives with polymer dopants such as polyacrylic acid, poly(L-aspartic acid-co-L,L-lactide), and inorganic acid $H_4SiW_{12}O_{40} \times 39 H_2O$.
 - Polyester hydrochlorides, synthesized from methyl- or octyldiethanolamine and various acid chlorides, were used for modification of montmorillonite (MMT). The interlayer spacing of modified MMT is influenced by the length of the side chain and not by the length of the acid residue.
 - Nanoparticles and nanowires of ZnO with particle sizes 20 - 100 nm were synthesized by the polyol method and used for the preparation of nanocomposites of poly(methyl methacrylate), PMMA. Nanocomposites are

- svetlobo in so termično bolj stabilni od PMMA.
- V sodelovanju z raziskovalci Instituta Jožef Stefan smo pripravili nanokompozite z visoko koncentracijo superparamagnetnih nanodelcev v matrici PMMA. Nanokompoziti ohranijo superparamagnetne lastnosti pri koncentraciji delcev do 48 %.
 - V sodelovanju s sodelavci iz Julona smo raziskali vpliv procesnih parametrov in dodatka kompatibilizatorja na porazdelitev poliamida 6 (PA6) v matrici polipropilena in na mehanske lastnosti. Velikost delcev PA6 pada s povečanjem koncentracije kompatibilizatorja do 8 %.
 - V sodelovanju s sodelavci iz Savatech, d.o.o., smo pripravili kompozite in nanokompozite iz kavčuka EPDM in polnila ZnO ali MMT. Raziskali smo vpliv procesnih parametrov na porazdelitev delcev v elastomerni matrici in na lastnosti vulkanizatov.
 - Na področju raziskav fotokatalitičnih samočistilnih premazov smo pripravili različne premaze z nanodelci titanovega dioksida transparent, effectively absorb UV light and thermally stabilize the PMMA matrix.
 - Nanocomposites with a high concentration of superparamagnetic particles in the PMMA matrix were prepared in collaboration with researchers from the Institute Jožef Stefan. Superparamagnetic properties of the nanocomposites are preserved at the concentration up to 48 %.
 - The influence of processing parameters and effect of compatibilizer on distribution of polyamide 6 (PA6) within the polypropylene matrix and on the mechanical properties were investigated in collaboration with Julon, d.d. The size of PA6 domains decreases with increasing content of the compatibilizer up to 8 %.
 - In collaboration with Savatech, d.o.o., we prepared composites and nanocomposites from EPDM rubber and filler ZnO or MMT. The influence of processing parameters on particle distribution and properties of vulcanisates were studied.



SLIKA 1:
Utrinki z otvoritve kongresa

FIGURE 1:
Moments from opening ceremony

(TiO₂) in izdelali laboratorijski UV reaktor, s katerim lahko primerjamo učinkovitost fotokatalitične aktivnosti posameznih formulacij.

- V sodelovanju z raziskovalci Kolpe smo raziskali možnosti uporabe kompozitnega akrilno-poliestrskega odpadka. Razvili smo postopek mešanja zmlatega odpadka z nenasičeno poliestrsko smolo, ki je bil uspešno preizkušen v proizvodnji pri industrijskem partnerju.
- Delo na uporabi odpadnega polietilentereftalata smo zaključili z razvojem postopka za sintezo dodatkov za preprečevanje skrčkov pri nenasičenih poliestrskih smolah. V dodatek smo vključili okoli 40% odpadnega PET ter dosegli minimalne skrčke, primerljive s komercialnimi dodatki.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Razvojni inštitut, Savatech, d.o.o., Kranj: sodelovanje pri raziskovalnem programu in projektu ter razvojno investicijskem projektu

- We prepared photocatalytic self-cleaning coatings, based on titanium dioxide (TiO₂). We have constructed a laboratory scale UV reactor where the photo-catalytic activity of different formulations can be measured.

- In collaboration of Kolpa, d.d., we studied the possibilities of recycling of a acrylic-polyester composite waste. We developed the process of binding the ground waste with an unsaturated polyester resin which was successfully tested in the production of our industrial partner.

- We finished the work on the use of waste poly(ethylene terephthalate) for resin and coatings production with development of simple procedure for the synthesis of low profile additives (LPA) for unsaturated polyester resins. We were able to include approximately 40 % of PET in LPA and achieve shrinkage results comparable to commercial products.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Research & Technology Institute, Savatech,



SLIKA 2:
Utrinki z otvoritve kongresa

FIGURE 2:
Moments from opening ceremony

- (ESRR) na področju elastomernih nanokompozitov;
- Julon, d.d., Ljubljana: sodelovanje pri razvojno investicijskem projektu (ESRR) »MTX – inovativno vlakno prihodnosti«;
 - Lek farmacevtska družba d.d., Ljubljana: raziskovalno-razvojno sodelovanje;
 - Color d.d, Medvode: sodelovanje pri aplikativnem projektu na področju uporabe odpadnega polietilentereftalata;
 - Kolpa d.d., Metlika: razvoj kadrov in razvoj postopkov ponovne uporabe industrijskih polimernih odpadkov;
 - KLI Logatec in Biotehniška fakulteta Univerze v Ljubljani: sodelovanje pri aplikativnem projektu na področju sinteze veziv in razvoja novih premaznih sistemov z nizko vrednostjo HOS za lesno industrijo;
 - Fakulteta za strojništvo, Univerza v Ljubljani, in Institut Jožef Stefan: raziskovalni projekt na področju polimernih nanokompozitov;
 - Institut Jožef Stefan: aplikativni projekt na področju uporabe visoko reaktivne plazme;
 - Tehnološka platforma Napredni materiali in tehnologije;
 - ZORD, Ljubljana: raziskovalno-razvojno sodelovanje;
 - Za različne partnerje iz industrije (Kolektor, Tekstilna tovarna Okroglica, itd.) analiziramo polimerne in druge materiale ter rešujemo strokovne probleme.
- d.o.o., Kranj, Slovenia: Elastomeric nanocomposites (research program and project, development and industrial project, European funds for regional development)
- Julon d.d., Ljubljana, Slovenia: MTX – innovative fiber for the future, development and industrial project, European funds for regional development
 - Lek, pharmaceuticals d.d., Ljubljana, Slovenia: research and development collaboration
 - Color d.d., Medvode, Slovenia: The application of waste polyethylene terephthalate (applied project)
 - Kolpa, d.d., Metlika, Slovenia: research and development collaboration
 - KLI Logatec and Biotechnical Faculty, University of Ljubljana, Slovenia: Binders and novel coatings systems with low content of VOC for wood industry (applied project)
 - Faculty of Mechanical Engineering, University of Ljubljana, and Jožef Stefan Institute, Ljubljana, Slovenia: Polymer-based nanocomposites (research project)
 - Jožef Stefan Institute, Ljubljana, Slovenia: Highly reactive plasma (applied project)
 - Technological platform Advanced Materials and Technologies
 - ZORD, Ljubljana, Slovenia: research and development cooperation
 - We analyze polymeric materials and solve professional problems for our industrial partners in Slovenia (Kolektor, Tekstilna tovarna Okroglica, ...)

MEDNARODNO SODELOVANJE

- Sodelovanje pri projektu 6.OP EU, 2006-2009, Nanoscale functionalities for targeted delivery of biopharmaceutics, akronim Nanobiopharmaceutics;
- sodelovanje pri mreži odličnosti, 6. OP EU, 2004-2008: Nanostructured and functional polymer-based materials and nanocomposites, akronim Nanofun-poly;
- Centre for Polymer and Carbon Materials, Zabrze, Poljska, Marie Curie Centre of Excel-

INTERNATIONAL COLLABORATION

- Participation in the Integrated Project, 6th EC Framework Program, 2006-2009: Nanoscale functionalities for targeted delivery of biopharmaceutics, acronym Nanobiopharmaceutics
- Network of Excellence, 6th Framework Program, 2004-2008: Nanostructured and functional polymer-based materials and nanoco-

lence: študijska izmenjava;

- ICS-UNIDO, Trst, Italija: sodelovanje na programu Applied Chemistry – Biodegradable plastics;
- bilateralna: Slovenija – Češka (Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Praga): Nanostrukturni polimerni kompozitni sistemi za uporabo v sončnih celicah in elektronskih napravah;
- bilateralna: Slovenija – Hrvaška (Fakultet kemijskog inženjerstva i tehnologije, Sveučilište u Zagrebu): Polimerni nanokompozitni materiali na osnovi montmorillonita.

POMEMBNI INŠTRUMENTI IN OPREMA

- Diferenčni dinamični kalorimeter Pyris 1, Perkin Elmer;
- FTIR spektrometer Spectrum One, Perkin Elmer;
- plinski kromatograf GC 8700, Perkin Elmer;
- souporaba plinskega kromatografa Hewlett Packard Agilent 6890N z masno selektivnim

mposites, acronym Nanofun-poly

- Centre for Polymer and Carbon Materials, Zabrze, Poland; invited researcher at the Marie Curie Centre of Excellence
- ICS-UNIDO, Trieste, Italy: collaboration at the programme Applied Chemistry – Biodegradable plastics
- Bilateral collaboration between Slovenia and Czech republic (Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague): Nanophase polymer-composite systems for solar cells and electronic devices
- Bilateral collaboration between Slovenia and Croatia (Faculty of Chemical Engineering and Technology, University of Zagreb): Polymer nanocomposites based on montmorillonites

MAJOR EQUIPMENT

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



SLIKA 3:

Otvoritveno predavanje Nobelovca prof. Jean-Marie Lehna

FIGURE 3:

Opening lecture of the Nobel laureate Prof. Jean-Marie Lehn

- detektorjem 5973N;
- tekočinski kromatograf z UV, RI (Perkin Elmer, Hewlett Packard) in ELS 2100 (Polymer Laboratories) detektorji za meritve SEC in dvodimenzionalne kromatografije;
- tekočinski kromatograf z detektorjem na sipanje svetlobe (Hewlett Packard, Wyatt Technology Corporation) za meritve SEC-MALS in SLS;
- suha komora Uni-Lab 1200780, M. Braun;
- souporaba SEM in STEM: vrstični elektronski mikroskop s poljsko emisijo FE-SEM SUPRA 35 VP, Carl Zeiss, z energijsko disperzivno spektroskopijo Inca 400 (Oxford Instruments);
- souporaba krio-ultramikrotoma Leica UC6/FC6;
- souporaba velike inštitutske opreme (NMR 300 MHz, 600 MHz in 800 MHz, WAXS, LC-MS);
- souporaba mikrovalovne pečice Milestone MLS 1200 Mega;
- dvopolžni laboratorijski ekstruder Teach-Line ZK 25T z vodno kopeljo in granulatorjem, Dr. Collin;
- stroj za injekcijsko vbrizgavanje Babyplast, Rambaldi+Co.
- 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 (Wyatt Technology Corp., USA), which can be used as a detector in SEC-MALS or independently for static light scattering measurements (SLS)
- Stainless steel glove-box system Uni-Lab 1200780, M. Braun
- Joint use of a microwave oven Milestone MLS 1200 Mega
- Joint use of large Institute's equipment (NMR 300 MHz, 600 MHz and 800 MHz, WAXS, LC-MS)
- Joint use of SEM and STEM: Field emission scanning electron microscope FE-SEM SUPRA 35 VP, Carl Zeiss, equipped with energy dispersive spectroscopy Inca 400 (Oxford Instruments)
- Joint use of krio-ultramikrotom Leica UC6/FC6
- Twin screw extruder Teach-Line ZK 25T with water bath and strand pelletizer, Dr. Collin
- Injection moulding machine Babyplast, Rambaldi+Co.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Mentorstva, komentorstva:

- Gregor Kočevar, strokovno izpopolnjevanje do magisterija;
- Judita Grm, mentorstvo pri diplomu visokošolskega študija;
- Davor Mihalić, komentorstvo pri diplomu visokošolskega študija;
- Boštjan Cesar, komentorstvo pri diplomu visokošolskega študija.

Obiski:

- Obiski v okviru bilateralnega sodelovanja: prof. dr. Jiri Vohlřdal, Charles University, Praga, Češka, mag. Ivan Brnardić, Univerza v Zagrebu, Hrvaška;

EDUCATION AND VISITS

Mentorship, comentorships:

- Gregor Kočevar, professional advanced study to master degree
- Judita Grm, mentorship at undergraduate studies
- Davor Mihalić, comentorship at undergraduate studies
- Boštjan Cesar, comentorship at undergraduate studies

- prof. dr. Brigitte Voit, Leibniz-Institut für Polymerforschung, Dresden, Nemčija;
- organizirali smo skupščino Evropske polimerne federacije.

EUROPEAN POLYMER CONGRESS 2007, Portorož, Slovenia, July 2-6, 2007

V dvoletnem obdobju 2005-2007 je Evropski polimerni federaciji, EPF, predsedovala prof. dr. Majda Žigon, zato je bila organizacija kongresa poverjena Sloveniji.

Evropski polimerni kongresi se uvrščajo med najbolj pomembne mednarodne dogodke na področju polimerov in potekajo vsako drugo leto pod pokroviteljstvom Evropske polimerne federacije (EPF, www.europolymer.org), ki združuje 29 polimernih društev iz 27 evropskih držav. Tokrat je bil Evropski polimerni kongres prvič v Sloveniji. Kongres je bil izrednega pomena za Slovenijo na področju znanstveno raziskovalnega dela na univerzah, raziskovalnih organizacijah in v gospodarstvu ter tudi za širšo promocijo Slovenije v svetu. Konferenca je bila po mnenju večine udeležencev izjemno uspešna in odmevna, tako po znanstveni kakovosti prispevkov kot tudi po organizaciji. Organizatorji Evropskega polimernega kongresa 2007 v Portorožu so bili Sekcija za polimere Slovenskega kemijskega društva, EPF, Kemijski inštitut, Univerza v Ljubljani in Univerza v Mariboru, sodelavci laboratorija pa so bili člani lokalnega organizacijskega odbora.

Evropski polimerni kongres je namenjen promociji raziskav na področju polimerov, pregledu najnovejših in najbolj zanimivih znanstvenih rezultatov ter komunikaciji med svetovno priznanimi znanstveniki, raziskovalci, študenti in drugimi udeleženci. Program kongresa je sestavljalo osem tematskih sklopov, od kemije in fizike polimerov, razvoja naprednih polimernih materialov za uporabo na različnih področjih, do modeliranja in simulacij ter predelave polimernih materialov. Kongresa EPF-2007 (<http://www.epf2007.org>) se je udeležilo 824 udeležencev iz 49 držav, velika večina

Visits:

- Visitors in the frame of bilateral collaboration: Prof. Dr. Jirí Vohlídal, Charles University, Prague, Czech republic; Ivan Brnardić, M. Sc., University of Zagreb, Croatia
- Prof. Dr. Brigitte Voit, Leibniz-Institut für Polymerforschung, Dresden, Germany
- Organization of the General Assembly meeting of the European Polymer Federation

EUROPEAN POLYMER CONGRESS 2007, Portorož, Slovenia, July 2-6, 2007

In the period 2005-2007 Prof. Majda Žigon was the president of the European Polymer Federation (EPF) which also meant that Slovenia became the host for the Congress.

European Polymer Congresses are biannual meetings, one of the year's most important events in polymer science and one of the major activities of the European Polymer Federation (EPF, www.europolymer.org), which is an independent association of 29 academic and industrial national organizations from 27 European countries, dealing with polymers. The 4th European Polymer Congress (www.epf2007.org) was held for the first time in Slovenia and was, according to the opinion expressed by many participants, a great success. The conference was organized by the Section for Polymers of the Slovenian Chemical Society, the European Polymer Federation, the National Institute of Chemistry, the University of Ljubljana, and University of Maribor, while the members of the Laboratory acted as Local Organizing Committee.

The EPF congresses aim to promote polymer research and to bring together polymer scientists, researchers, students, and other relevant participants. They overview both state of the art as well as new initiatives in already established and emerging fields of polymer science and technology. The scientific programme of the conference covered the chemistry and physics of polymers, modeling and simulation, and the processing of polymers and polymeric ma-

udeležencev, kar 85 %, je bila iz Evrope. Največ udeležencev je bilo iz Slovenije in Nemčije, sledile so Francija, Italija, Rusija, Španija, Poljska, Romunija, Nizozemska in druge. Na kongresu je bilo 15 plenarnih in 90 vabljenih predavanj vrhunskih znanstvenikov s področja polimerov, med njimi je bilo sedem slovenskih predavateljev in svetovno znani Nobelov nagrajenec za kemijo leta 1987, prof. dr. Jean-Marie Lehn iz Francije. Organizirana je bila tudi okrogla miza o visokošolskem izobraževanju na področju polimerov v nekaterih evropskih državah z vidika prednosti in pomanjkljivosti bolonjskega procesa. Ob znanstvenem delu kongresa so lahko udeleženci uživali v sproščeni atmosferi ob večeru dobrodošlice, večerji za vabljene predavatelje, slavnostni večerji in poslovnem pikniku s slovensko etnoskupino Terrafolk, ob tej priložnosti pa so bile podeljene nagrade za najboljše posterje dvanajstim mladim raziskovalcem.

Posebna zahvala gre našim glavnim sponzorjem: Smile Group (Nizozemska), Julon d.d., Ljubljana, Helios d.d., Domžale in Savi d.d., Kranj ter Ministrstvu za visoko šolstvo, znanost, in tehnologijo RS, Javni agenciji za raziskovalno dejavnost RS, založbi Elsevier in Kemijskemu inštitutu.

materials, which were covered in the eight sessions. There were 824 participants and 49 countries were represented. The majority of participants (85 %) were from Europe with the highest number from Slovenia and Germany, followed by France, Italy, Russia, Spain, Poland, Romania, the Netherlands, and other countries. The program included 15 plenary and 90 invited lectures of top scientists from the polymer field. Among these were seven Slovenian lecturers and world known Nobel prize winner, Prof. Dr. Jean-Marie Lehn. In addition, a round table discussion on polymer education was organized providing some observations on the advantages and drawbacks of implementing the Bologna process in different European countries.

Apart from scientific work, the participants enjoyed a more relaxed atmosphere in the evenings at the welcome reception, dinner for invited speakers, gala dinner, and the farewell party, which featured the popular Slovenian band Terrafolk, while twelve young researchers were awarded for the best poster presentations.

Special thanks go to the industrial sponsors: Smile Concepts Group, the Netherlands; Julon, d.d., Ljubljana; Helios d.d., Domžale; Sava d.d., Kranj and Savatech, Kranj, (all from Slovenia), as well as to the Slovenian Ministry of Higher Education, Science and Technology, Slovenian Research Agency, publisher Elsevier and the National Institute of Chemistry.

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

Miha Steinbacher (od novembra / from November)

**MLADI RAZISKOVALEC /
YOUNG RESEARCHER**

Damjan Šterk

Borut Zupančič

Matjaž Brvar (od oktobra / from October)



PODROČJA DEJAVNOSTI

- Razvoj novih metodologij v asimetrični sintezi in homogeni katalizi;
- sinteza optično aktivnih spojin s potencialno biološko aktivnostjo;
- raziskave in razvoj novih sintetskih poti do industrijsko uporabnih spojin

<http://www.ki.si/index.php?id=180>

BIBLIOGRAFIJA

- 1 izvorni znanstveni članek
- 1 samostojni znanstveni sestavek v monografiji
- 1 patentna prijava
- 1 uredništvo revije

GLAVNI DOSEŽKI V LETU 2007

Asimetrično transfer hidrogeniranje

Priprava kiralnih alkoholov in aminov na osnovi industrijsko uporabne tehnologije bazirajoče na uporabi mravljinčne kisline-trietilamina in naših rutenijevih kompleksov [Ru(aren)(S,S)-R₂NSO₂DPEN]. Različni razredi ketonov (alfa-arilirani, alfa-/beta-acetilenski, fluoroalkil idr.) so bili uspešno reducirani v visokih enantiomernih presežkih in visokih izkoristkih z uporabo

RESEARCH ACTIVITIES

- Development of new methodologies in asymmetric synthesis and homogeneous catalysis
- Synthesis of optically active compounds of potential biological activities
- Research and development of new synthetic routes towards industrially interesting compounds

<http://www.ki.si/index.php?id=180&L=1>

BIBLIOGRAPHY

- 1 Original Scientific Article
- 1 Independent Scientific Component Part in a Monograph
- 1 Patent Application
- 1 Journal Editorship

IMPORTANT ACHIEVEMENTS IN 2007

Asymmetric transfer hydrogenation

Preparation of chiral alcohols and amines relying on industrially useful technology based on use of formic acid-triethylamine and our ruthenium based [Ru(arene)(S,S)-R₂NSO₂DPEN] complexes. A variety of classes of ketones (alpha-arylated, alpha-/beta-acetylenic, fluoroalkyl, etc) were successfully reduced in high enantio-

tovrstnih novih Ru-kompleksov. Poleg tega so bili naši kompleksi uporabljeni pri sintezi različnih farmacevtskih intermediatov.

Asimetrično hidrogeniranje

Priprava optično aktivnih alfa- ali beta-aminokislin, aminov, alkoholov in njihovih derivatov na osnovi industrijsko uporabne tehnologije bazirajoče na uporabi vodika in naših rodijevih katalizatorjev s P-stereogenimi difosfinskimi ligandi. Pripravljene so bile različne družine takšnih ligandov, kar omogoča bolj učinkovito pripravo željenih optično aktivnih intermediatov.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

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

meric excesses and high yields using our new Ru-complexes. In addition, our complexes were explored in the synthesis of several pharmaceutical intermediates.

Asymmetric hydrogenation

Preparation of optically active alpha- or beta-aminoacids, amines, alcohols, and their derivatives relying on industrially useful technology based on use of hydrogen and our rhodium-based P-stereogenic diphosphine ligand complexes. A large variety of families of these ligands were prepared allowing more efficient preparation of the desired optically active intermediates.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Krka Pharmaceuticals, d.d., Novo mesto, Slovenia: Development of new synthetic routes to selected pharmaceutical intermediates;
- Lek Pharmaceuticals, d.d., Ljubljana, Slovenia: Synthesis of potential pharmaceutical compounds;



SLIKA 1:
Merjenje optične rotacije

FIGURE 1:
Measurement of optical rotation

MEDNARODNO SODELOVANJE

- COST-D40 Inovativni katalizatorji: Novi procesi in stereoselektivnosti

- PhosPhoenix SARL, Paris, France: Development of industrial processes based on homogeneous catalysis.

POMEMBNI INSTRUMENTI IN OPREMA

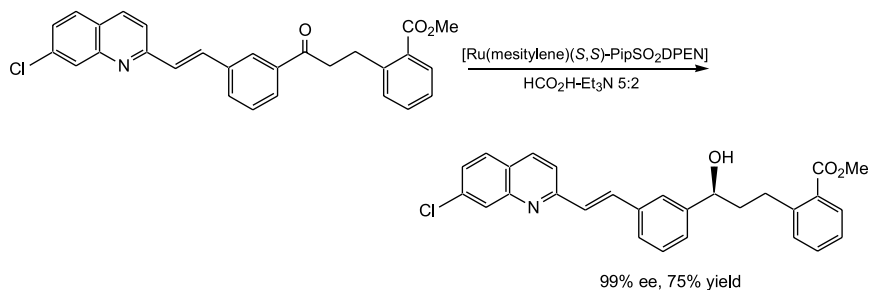
- HPLC in GC sistemi opremljeni s kiralnimi kolonami
- Polarimeter
- Ultra kriomat (-100 do +100 °C)
- Sistem za hidrogeniranje (do 100 atm H₂)

INTERNATIONAL COLLABORATION

- COST-D40 Action Innovative Catalysts: New Processes and Selectivities

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)



HEMA 1

Asimetrično transfer hidrogeniranje intermedija za farmacevtsko učinkovino Montelukast

SCHEME 1

Asymmetric transfer hydrogenation of Montelukast pharmaceutical ingredient

L09

Laboratorij za anorgansko kemijo
in tehnologijo

Laboratory for Inorganic Chemistry
and Technology



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Edi Kranjc



PODROČJA DEJAVNOSTI

Raziskave poroznih materialov:

- zeolitni materiali
- mezoporozni materiali
- cement

Strukturna analiza materialov:

- rentgenska difrakcija
- nuklearna magnetno resonančna spektroskopija
- rentgenska absorpcijska spektroskopija

BIBLIOGRAFIJA

- 9 izvirnih znanstvenih člankov
- 1 kratki znanstveni prispevek
- 1 strokovni članek
- 1 samostojni strokovni sestavek v monografiji
- 2 objavljena znanstvena prispevka na konferencah (vabljeni predavanja)
- 2 objavljena znanstvena prispevka na konferencah
- 15 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 predavanje na tuji univerzi

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

- 9 Original Scientific Articles
- 1 Short Scientific Article
- 1 Professional Article
- 1 Independent Professional Component Part in a Monograph
- 2 Published Scientific Conference Contributions (Invited Lectures)
- 2 Published Scientific Conference Contributions
- 15 Published Scientific Conference Contribution Abstracts
- 1 Invited Lecture at Foreign University
- 1 Unpublished Invited Conference Lecture

- 1 vabljen predavanje na konferenci brez natisa
- 1 končno poročilo o rezultatih raziskav
- 2 diplomi
- 3 uredništva revij

GLAVNI DOSEŽKI V LETU 2007

- Priprava s titanom modificiranih zeolitnih delčkov nanometerskih velikosti

Vgrajevanje prehodnih kovin v zeolitne delčke nanometerskih velikosti poteka po še ne v celoti raziskanih mehanizmi v primerjavi z vgrajevanjem prehodnih kovin v zeolitne kristale mikrometerskih velikosti. Raziskovali smo mehanizem vgrajevanja titana. Zeolitni delčki nanometerskih velikosti so ključni za pripravo katalizatorjev s hierarhično porozno strukturo kot tudi za pripravo tankih filmov.

- Razvoj titanovih katalizatorjev s hierarhično porozno strukturo

S prehodnimi kovinami modificirane mikroporozne silikate (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 ter narave vgrajene kovine in njenega mesta vgradnje v ogrodje. Mezoporozni silikati (premer por od 2 do 10 nm) omogočajo udeležbo v katalitskih reakcijah tudi molekulam večjih dimenzij, vendar je njihova temperaturna stabilnost slabša in ne dosegajo katalitskih lastnosti mikroporoznih silikatov. Naše raziskave so bile usmerjene v pripravo novih katalizatorjev s hierarhično porozno strukturo, ki združujejo dobre katalitske lastnosti in temperaturno stabilnost mikroporoznih ter dimenzije por mezoporoznih materialov. Sintetizirali smo s titanom modificirane silikate s hierarhično porozno strukturo. Mikroporozno in mezoporozno strukturo smo raziskali z rentgensko difrakcijo in transmisijskim

- 1 Final Research Report
- 2 Undergraduate Theses
- 3 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2007

- Preparation of titanium-modified zeolitic nanoparticles

The incorporation mechanism of transition metals into small zeolitic particles has not yet been defined if compared to incorporation mechanism into crystalline zeolitic particles. We studied the incorporation mechanism of titanium. Zeolitic nanoparticles are essential for the preparation of catalysts having hierarchical porous structure and thin films.

- Development of titanium catalysts having hierarchical porous structures

Transition-metal modified microporous silicates (zeolites) with pore openings from 0.5 to 2 nm are widely used as heterogeneous catalysts in oxidation reactions. These catalysts exhibit remarkable catalytic activity due to transition-metal centers that are isolated in the silicate framework. Catalytic properties of these materials depend on the structure type, location and the nature of incorporated metal. The pore size limitations of microporous catalysts can be overcome by using mesoporous silicates with pore openings from 2 to 10 nm when larger reactants have to be processed. However, mesoporous species do not exhibit excellent catalytic properties and hydrothermal stability of microporous silicates. Our research was focused on the preparation of novel catalysts with hierarchical porous structure that combine good catalytic properties and thermal stability of microporous- and pore openings of mesoporous silicates. We have synthesized titanium-modified silicates with hierarchical porous structure. Microporous and mesoporous structures were investigated by X-ray powder diffraction and High Resolution Transmission Electron Microscopy. Local

mikroskopom z visoko ločljivostjo. Lokalno okolico titana v silikatnem ogrodju smo določili z rentgensko absorpcijsko spektroskopijo.

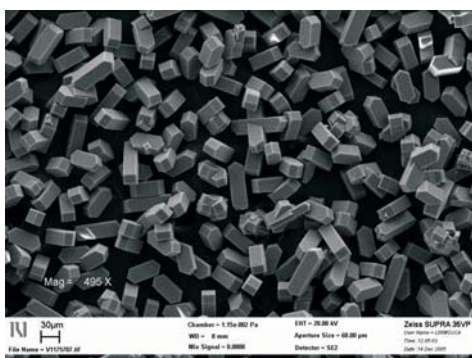
- Razvoj nove NMR metode za merjenje razdalj med kvadrupolnimi jedri

Z jedrsko magnetno resonanco smo pomagali karakterizirati mezoporozne aluminofosfate in mikro-mezoporozne silikatne kompozitne materiale. Razvili smo novo metodo za študij korelacij med dipolno sklopljenimi kvadrupolnimi jedri, npr. med jedri aluminija v aluminofosfatih, ki uporablja močna radiofrekvenčna polja. Mehanizem delovanja metode ni povzet po metodah za preprostejše sisteme sklopljenih jeter s spinom $1/2$, temveč je specifičen za kvadrupolna jedra. Z magnetno resonanco smo študirali tudi zgradbo zanimivih litijevih spojin, ki bodo v bodoče lahko izboljšale lastnosti litijevih baterij, in sistematično raziskovali spreminjanje kemijskega premika vodikovega jedra in kemijskega premika in kvadrupolne sklopitvene konstante devterijevega jedra v prisotnosti različno močnih vodikovih vezi.

- Uporaba zeolitnih adsorbentov za odstranjevanje arzena v postopkih priprave pitne vode

environment of the titanium in the silicate framework was identified by X-ray absorption spectroscopy.

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



a)

SLIKA 1:

Mikrografa zeolitov na vrstičnem elektronskem mikroskopu a) zeolitni kristali mikrometrskih velikosti, b) zeolitni delci nanometerskih velikosti



b)

FIGURE 1:

Scanning electron micrographs: a) crystalline zeolitic particles of micrometer size, b) zeolite nanoparticles

Naravne zeolite uporabljajo pri odstranjevanju amoniaka in težkih kovin iz odpadnih in pitnih vod. V sodelovanju z Univerzo v Zagrebu smo določili adsorpcijske karakteristike zeolitov iz Vranjske Banje (Srbija) in Donjega Jesenja (Hrvaška) za odstanjevanja arzena iz pitne vode. Karakteristike zeolitov smo študirali s pomočjo metode rentgenske difrakcije na praškastih vzorcih ter komplementarnih analitskih metod kot sta rentgenska absorpcijska spektroskopija in elektronska mikroskopija.

- Priprava okolju prijaznega cementa: Študij hidratacije cementa z mineralnimi dodatki Elektrofiltrskemu pepelu, ki je ena od mineralnih komponent pri hidrataciji ternarnega sistema cement-apnenec-pepel, smo določili kemijsko-fizikalne lastnosti, ki so pomembne za ustrezno formulacijo izhodnih mešanic. Preiskali smo reakcije med pepelom in apnencem v procesu hidratacije ter ugotovili, da je zaradi slabe reaktivnosti potrebno pepel kemijsko aktivirati. Reakcija med pepelom ter apnencem je odvisna od granulacije apnenca ter od časa hidratacije.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Silkem, Kidričevo: raziskave sintetičnih zeolitov in njihove aplikacije;
- Salonit, Anhovo d.d., Deskle: raziskave in razvoj okolju prijaznih cementov;
- Krka, d.d., Novo mesto: strukturne določitve in analize površin farmacevtskih produktov.

MEDNARODNO SODELOVANJE

- Projekt šestega okvirnega programa Evropske unije (2004-2008), INSIDE-PORES Network of Excellence - nosilec: prof. dr. Venčeslav Kaučič;
- ESRR – Evropski sklad za regionalni razvoj (2004-2007), Nanoscience and nanotechnology centre of excellence, Characterization on nanometric scale - nosilec: dr. Miran Čeh;

water treatment: Study of arsenic removal

Natural zeolites have been used for the removal of ammonia and heavy metals from drinking water and wastewaters. In collaboration with the University of Zagreb we determined the adsorption characteristics of zeolites from Vranjska Banja (Serbia) and Donje Jesenje (Croatia) for the arsenic removal from drinking water. Characteristics of zeolites were studied by using X-ray powder diffraction methods and complementary methods such as X-ray absorption spectroscopy and electron microscopy.

- Preparation of environment-friendly cement: Study of hydration of cement containing mineral admixtures

Fly ash that represents one of the components in a ternary system comprising portland cement, limestone and fly ash was characterized and chemical-physical properties that are necessary for the correct formulation of starting mixtures were determined. We ascertained that the reactivity of fly ash was low and that chemical activation was necessary. The hydration reaction between fly ash and limestone was influenced by both limestone granulation and hydration time.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Silkem, Kidričevo, Slovenia: investigations of synthetic zeolites and their applications
- Salonit Anhovo, d.d., Deskle, Slovenia: investigations and development of environment-friendly cements
- Krka d.d., Novo mesto, Slovenia: structural determinations and texture analyses of pharmaceutical products

INTERNATIONAL COLLABORATION

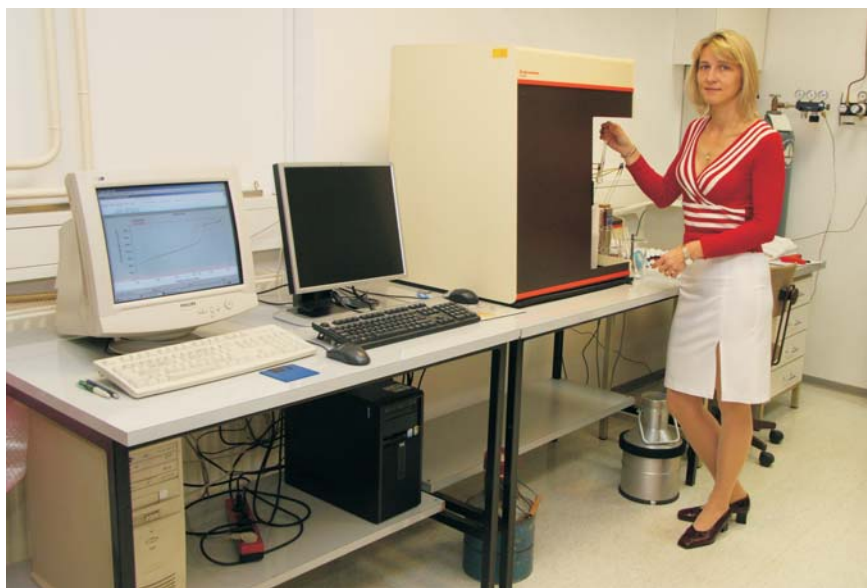
- INSIDE-PORES Network of Excellence (2004-2008), NoE 6th Framework Project EU - Principal investigator: Prof. Dr. Venčeslav Kaučič

- ESRR – Evropski sklad za regionalni razvoj (2004-2007), NMR centre of excellence, Study of structures and interactions in biotechnology and pharmacy -nosilec: prof. dr. Janez Plavec;
 - COST D 19 Chemical Functionality Specific to the Nanometer Scale - nosilec: prof. dr. Venčeslav Kaučič;
 - COST D 36 Molecular Structure-Performance Relationships at the Surface of Functional Materials - nosilec: prof. dr. Venčeslav Kaučič;
 - slovensko-argentinski bilateralni projekt (2006-2008): Modified Mesoporous Oxides – nosilec: prof.dr. Venčeslav Kaučič;
 - slovensko-srbski bilateralni projekt (2006-2007): By Rational Synthesis towards Smart Materials – nosilec: prof. dr. Venčeslav Kaučič;
 - slovensko-norveški bilateralni projekt (2007-2009): Smart Porous Composite Materials – nosilec: prof. dr. Venčeslav Kaučič;
 - PROTEUS (2007-2008) Hierarchical Nanoporous Catalysts: Synthesis, Characterization and Catalytic Performances – nosilka: doc. dr. Nataša Novak Tušar;
 - eksperimentalni projekti na sinhrotronu ELETTRA (2006600, 2007356) XAS studies of Ti, V, Mn and Fe local environment of hierarchical porous catalysts – nosilka: doc. dr. Nataša Novak Tušar;
 - PARTNERSHIP IN SCIENCE 2007 – Structural Properties of Metal-Organic Frameworks as Potential Hydrogen Storage Materials - nosilka: doc. dr. Nataša Zabukovec Logar;
 - slovensko-madžarski bilateralni projekt (2006-2007): Characterization of Iron Modified Nanoporous Silicates - nosilka: dr. Alenka Ristić.
 - ERDF - The European Regional Development Fund (2004-2007), Nanoscience and nanotechnology centre of excellence, Characterization on nanometric scale – Principal investigator: Dr. Miran Čeh
 - ERDF – The European Regional Development Fund (2004-2007), NMR centre of excellence, Study of structures and interactions in biotechnology and pharmacy - Principal investigator: Prof. Dr. Janez Plavec
 - COST D 19 Chemical Functionality Specific to the Nanometer Scale - Principal investigator: Prof. Dr. Venčeslav Kaučič
 - COST D 36 Molecular Structure-Performance Relationships at the Surface of Functional Materials - Principal investigator: Prof. Dr. Venčeslav Kaučič
 - Slovenia-Argentina bilateral project (2006-2008) Modified Mesoporous Oxides – Principal investigator: Prof. Dr. Venčeslav Kaučič
 - Slovenia-Serbia bilateral project (2006-2007) By Rational Synthesis towards Smart Materials – Principal investigator: Prof. Dr. Venčeslav Kaučič
 - Slovenia-Norway bilateral project (2007-2009) Smart Porous Composite Materials – Principal investigator: Prof. Dr. Venčeslav Kaučič
 - PROTEUS (2007-2008) Hierarchical Nanoporous Catalysts: Synthesis, Characterization and Catalytic Performances – Principal investigator: Dr. Nataša Novak Tušar, Assist. Prof.
 - Synchrotron ELETTRA experimental projects (2006600, 2007356) XAS studies of Ti, V, Mn and Fe local environment of hierarchical porous catalysts – Principal investigator: Dr. Nataša Novak Tušar, Assist. Prof.
 - PARTNERSHIP IN SCIENCE 2007 – Structural Properties of Metal-Organic Frameworks as Potential Hydrogen Storage Materials – Principal investigator: Dr. Nataša Zabukovec Logar, Assist. Prof.
- POMEMBNI INŠTRUMENTI IN OPREMA**
- 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 Johanssonovim monokromatorjem za vzorce z ravno površino, (2) kapilarna transmisija z hibridnim monokromatorjem, (3) standardna Bragg-Brentano, (4) paralelni žarek;
- 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;
 - 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
- Slovenia-Hungary bilateral project (2006-2007) Characterization of Iron Modified Nanoporous Silicates – Principal investigator: Dr. Alenka Ristić

MAJOR EQUIPMENT

- 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.
- 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



SLIKA 2:

Mojca Opresnik med meritvami na avtomatskem plinskem analizatorju za določanje specifične površine, adsorpcijskih izoterm, volumna in porazdelitve por praškastih vzorcev

FIGURE 2:

Mojca Opresnik performing a measurement on an automated gas adsorption analyser for the determination of specific surface area, adsorption isotherms, pore volume and pore size distribution of powder samples

simultane meritve energijskega pretoka in masnih sprememb v materialih od sobne temperature do 1500°C;

- Microtrac S3500, aparatura za določevanje velikosti in porazdelitev delcev v mokrem ali suhem stanju. Območje meritev za mokre vzorce od 0,02 μm do 1400 μm in za suhe vzorce od 0,25 μm do 1400 μm ;
- AutoPycnometer (Micromeritics Instrument Co.) aparatura za avtomatsko določevanje gostote materialov s helijem;
- Centrifuga Hettich, Rotanta 460 R hlajena (temperaturno območje od -20°C do $+40^{\circ}\text{C}$). Hitrost vrtenja od 500 do 9500 obr/min;
- Ultra Turrax disperzer T25 (IKA);
- Mikrovalovna peč MLS-1200 MEGA (Milestone);
- Mikrovalovna peč ETHOS (Milestone);
- Mlin za mešanje in homogeniziranje prahov, suspenzij in past Retsch RM 100;
- Kalcinacijske peči: dve cevni (segrevanje do 1000°C , hitrost segrevanja $1,5\text{-}2^{\circ}\text{C}/\text{min}$) in ena komorna (segrevanje do 1200°C , hitrost segrevanja $3^{\circ}\text{C}/\text{min}$).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Izobraževanje:

- Alja Lipovšek: diplomsko delo z naslovom »Sinteza mikroporoznega vanadijevega silikalita«, komentor: prof. dr. Venčeslav Kaučič;
- Alen Kljajić: diplomsko delo z naslovom »Sinteza antimonovih mezoporoznih silikatov«, komentor: prof. dr. Venčeslav Kaučič, Prešernova nagrada FKKT za diplomsko delo;
- dr. Gregor Mali je bil izvoljen v naziv docent za področje fizike na Univerzi Nova Gorica.

Obiski tujih raziskovalcev:

- dr. Franck Launay, University Pierre and Marie Curie, Paris, Francija;
- Sami Habib, University Pierre and Marie Curie, Paris, Francija;

or other atmospheres and for measurements of thin films.

- 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 30 to 1500°C).
- Microtrac S3500 Particle Size Analyzer, wet or dry samples. The range of measurement for wet samples is from 0.02 μm to 1400 μm (2800 μm) and for dry samples from 0.25 μm to 1400 μm .
- AutoPycnometer (Micromeritics Instrument Co.) for automatic determination of true density of materials with helium.
- High-speed centrifuge, Hettich, Rotanta 460 R, refrigerated (temperature control -20°C to $+40^{\circ}\text{C}$). Speed control within a range of 500 - 9.500 min^{-1} .
- Ultra Turrax disperser T25 (IKA).
- Microwave oven MLS-1200 MEGA (Milestone).
- Microwave oven ETHOS (Milestone).
- Grinder for mixing and homogenizing powders, suspensions and pastes, Retsch RM 100.
- Furnaces: two tubes (heating up to 1000°C , heating rate $1.5\text{-}2^{\circ}\text{C}/\text{min}$) and one chamber (heating up to 1200°C , heating rate $3^{\circ}\text{C}/\text{min}$).

EDUCATION AND IMPORTANT VISITS

Education:

- Alja Lipovšek: ended diploma thesis entitled »Synthesis of microporous vanadium silicalite«, co-mentor: Prof. Venčeslav Kaučič;
- Alen Kljajić: ended diploma thesis entitled »Synthesis of antimony mesoporous silicates«, co-mentor: Prof. Venčeslav Kaučič,

- dr. Madelaine Helliwell, University of Manchester, Manchester, Velika Britanija;
 - prof. Nevenka Rajić, Tehnološko-metalurška fakulteta, Univerza v Beogradu, Srbija;
 - prof. dr. Štefica Cerjan Stefanović, Fakulteta za kemijsko inženjerstvo in tehnologijo, Zagreb, Hrvaška;
 - mag. Karmen Margeta, Fakulteta za kemijsko inženjerstvo in tehnologijo, Zagreb, Hrvaška;
 - Mario Šiljeg, Fakulteta za kemijsko inženjerstvo in tehnologijo, Zagreb, Hrvaška.
- Gostovanja:
- prof. dr. Venčeslav Kaučič je gostoval na Unidad de Actividad Quimica, Buenos Aires, Argentina (3 tedne);
 - Saša Cecowski je gostovala na Unidad de
- awarded with Faculty Prešeren Prize;
 - Dr. Gregor Mali: was elected Assistant Professor for the field of physics at University of Nova Gorica, Slovenia.
- Visits of foreign researchers:
- Dr. Franck Launay, University Pierre and Marie Curie, Paris, France;
 - Sami Habib, University Pierre and Marie Curie, Paris, France;
 - Dr. Madelaine Helliwell, University of Manchester, Manchester, UK;
 - Prof. Nevenka Rajić, Tehnološko-metalurški fakultet, University of Belgrade, Serbia;
 - Prof. Dr. Štefica Cerjan Stefanović, Fakultet kemijskog inženjerstva i tehnologije Sveučilišta u Zagrebu, Zagreb, Croatia;



SLIKA 3:
Edi Kranjc med meritvami na rentgenskem praškovnem difraktometru za identifikacijo in določanje strukture praškastih vzorcev

FIGURE 3:
Edi Kranjc performing a measurement on X-ray powder diffractometer for the identification and determination of structure of powdered samples

- Actividad Quimica, Buenos Aires, Argentina (6 mesecev);
- doc. dr. Gregor Mali je gostoval na Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, Francija (1 mesec);
 - doc. dr. Nataša Novak Tušar je gostovala na Univerzi Pierre in Marie Curie, Paris, Francija (1 teden);
 - Matjaž Mazaj je gostoval na Univerzi Pierre in Marie Curie, Paris, Francija (1 teden);
 - doc. dr. Nataša Novak Tušar je gostovala na Tehnološko-metalurški fakulteti, Univerza v Beogradu, Srbija, (1 teden).
- Msc. Karmen Margeta, Fakultet kemijskog inženjerstva i tehnologije Sveučilišta u Zagrebu, Zagreb, Croatia;
 - Mario Šiljeg, Fakultet kemijskog inženjerstva i tehnologije Sveučilišta u Zagrebu, Zagreb, Croatia.
- Visits of foreign institutes:
- Prof. Dr. Venčeslav Kaučič visited Unidad de Actividad Quimica, Buenos Aires, Argentina (3 weeks);
 - Saša Cecowski visited Unidad de Actividad Quimica, Buenos Aires, Argentina (6 months);
 - Dr. Gregor Mali, Assist. Prof., visited Lavoisier Institute, Versailles-Saint-Quentin-en-Yvelines University, Versailles, France (1 month);
 - Dr. Nataša Novak Tušar, Assist. Prof. visited University Pierre and Marie Curie, Paris, France (1 week);
 - Matjaž Mazaj visited University Pierre and Marie Curie, Paris, France (1 week);
 - Dr. Nataša Novak Tušar, Assist. Prof., visited Tehnološko-metalurški fakultet, University of Belgrade, Serbia (1 week).

L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry



VODJA / HEAD
doc. dr. Janko Jamnik

RAZISKOVALCI / RESEARCHERS

dr. Marjan Bele
dr. Robert Dominko
doc. dr. Miran Gaberšček

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Boštjan Erjavec
Boštjan Genorio
Aljaž Godec (od / from 01. 10. 2007)
Mirjana Kuzma
Jože Moškon
Dušan Strmčnik (do / until 30. 06. 2007)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Milena Zorko
Gregor Kapun



PODROČJA DEJAVNOSTI

- Materiali za energijske in informacijske tehnologije

Podrobnejša opredelitev:

- študij kinetike transporta in sprememb kemijske sestave v trdnih mešanih prevodnikih;
- vpliv nanostrukturiranosti trdnih kompozitov na izbrane lastnosti, kot so elektrokemijsko shranjevanje energije, raztapljanje, elektrokataliza ipd. (uporaba v energetiki, informatiki, farmaciji);
- priprava nanometrskih filmov na zunanjih in/ali notranjih površinah funkcionalnih materialov;
- priprava in karakterizacija novih nanostrukturiranih materialov za litijeve baterije;
- vgradnja funkcionalnih materialov v ustrezne matrice.

BIBLIOGRAFIJA

- 23 izvirnih znanstvenih člankov
- 1 strokovni članek
- 1 poljudni članek
- 2 intervjuja

RESEARCH ACTIVITIES

- Materials for energy and information technologies

Detailed classification:

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

BIBLIOGRAPHY

- 23 Original Scientific Articles
- 1 Professional Article
- 1 Popular Article

- | | | | |
|----|--|----|--|
| 1 | drugo učno gradivo | 2 | Interviews |
| 3 | objavljeni znanstveni prispevki na konferencah (vabljeni predavanja) | 1 | Other Educational Material |
| 14 | objavljenih povzetkov znanstvenih prispevkov na konferencah | 3 | Published Scientific Conference Contributions (Invited Lectures) |
| 1 | patent | 14 | Published Scientific Conference Contribution Abstracts |
| 2 | predavanja na tujih univerzah | 1 | Patent |
| 1 | končno poročilo o rezultatih raziskav | 2 | Invited Lectures at Foreign Universities |
| 5 | elaboratov, predštudij, študij | 1 | Final Research Report |
| 2 | diplomi | 5 | Treatises, Preliminary Studies, Studies |
| 1 | magisterij | 2 | Undergraduate Theses |
| 1 | doktorat | 1 | Master's Thesis |
| | | 1 | Doctoral Dissertation |

GLAVNI DOSEŽKI V LETU 2007

Transport naboja v litijevih baterijah: nov empirični zakon

V zadnjih letih so raziskovalci izumili številne nove katodne materiale za litijeve baterije, ki kažejo zelo visoke kapacitete, hkrati pa so tudi varni in poceni. Skoraj vsi pa imajo najmanj eno izrazito slabost: zelo nizko elektronsko prevodnost (pod 10^{-10} S/cm). Ker je prevajanje elektronov ključnega pomena za delovanje baterije, težavo poskušamo rešiti tako, da pripravimo zelo majhne delce (premera nekaj deset nanometrov) in nato vsak posamezen delec pripnemo na elektronski prevodnik, ki vodi do elektronskega izvora (postopek imenujemo elektronsko ožičenje). Enako moramo storiti tudi v litijevimi ioni (ionsko ožičenje). V praksi elektronsko ožičenje največkrat izvedemo tako, da vsak aktivni delec prekrijemo z nekaj nanometrov debelim slojem prevodnega ogljika. Za ionsko ožičenje pa poskrbi tekoči elektrolit, ki ga nalijemo v pore med aktivnimi delci. Doslej je med raziskovalci baterij trdno veljala domneva, da je elektronsko ožičenje precej pomembnejše od ionskega, saj naj bi bila elektronska prevodnost vseh omenjenih materialov precej slabša od ionske. Merilo za kvaliteto elektronskega ožičenja naj bi bila homogenost ogljikovega nanometerskega filma: bolj homogeni filmi naj bi zagotavljali boljše ožičenje in s tem manjše izgube pri uporabi baterij.

IMPORTANT ACHIEVEMENTS IN 2007

Transport of charge in lithium batteries: a new empirical law

During recent years, many novel high capacity, safe and cheap cathode materials for lithium batteries have been discovered. Basically all of them, however, exhibit at least one major drawback: an extremely low electronic conductivity (below 10^{-10} S/cm). As electron conduction is crucial for battery operation, the low-conductivity material is usually prepared in a form of small particles (several tens of nanometres in diameter), then each such tiny particle is connected to an electronic wire leading to an electron source (the procedure is termed electronic wiring). A similar procedure is then used to connect the particles to an ionic source (ionic wiring). In practice, the electronic wiring is realized by covering each active particle with a nanometre-thick film of conductive carbon. The ionic wiring, however, is carried out by pouring a liquid electrolyte in the spaces between the active particles. Until now, the battery researchers have strongly believed that the electronic wiring is much more important than the ionic because the inherent electronic conductivity of all materials has been assumed to be much lower than the ionic. A common measure for the quality of electronic has been the homogeneity of the conductive carbon film: the more homogeneous the film the better the elec-

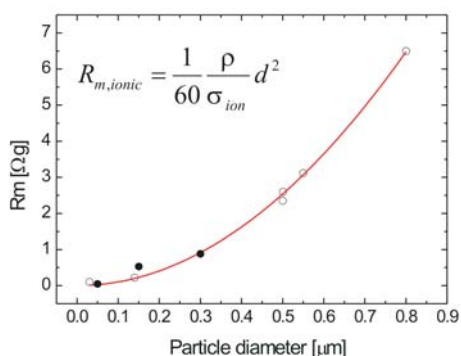
V laboratoriju smo na osnovi skrbne analize številnih literaturnih podatkov in lastnih meritev na modelskem fosfatnem materialu pokazali, da je elektronsko ožičenje pravzaprav precej manj pomembno od ionskega. Skonstruirali smo eksperimentalni graf, ki kaže odvisnost elektrodne upornosti od velikosti aktivnih delcev. Analiza je pokazala, da odvisnost skoraj natančno ustreza kvadratnemu zakonu, ne glede na kvaliteto elektronskega ožičenja. Z modeliranjem na kontinuum nivoju smo pokazali, da v tem primeru kvadratni zakon dobimo le, če je ionska prevodnost aktivnega delca precej manjša od elektronske. Skoraj istočasno z objavo naših ugotovitev je skupina z inštituta Max-Planck v Stuttgartu objavila eksperimentalne meritve, ki kažejo, da je pri visokih temperaturah ionska prevodnost fosfatnega materiala resnično manjša od elektronske (meritve pri sobnih pogojih zaenkrat žal niso izvedljive), kar je povsem v skladu z našimi opažanji.

Naše ugotovitve bodo predvidoma imele pomembne vpliv na bodoče načrtovanju nanoarhitekture baterijskih elektrod. Potrebno bo več pozornosti posvetiti zmanjševanju aktivnih delcev, med katerimi bo vsaj nekaj praznega prostora, v katerega bomo lahko nalili elektrolit in s tem kvalitetno ionsko ožičili vsak posamezni delec. Obenem bo potrebno sicer

tronic wiring and the better the cathode performance.

Based on a number of careful analyses of literature data and on our own experimental results on a model phosphate electrode, we have demonstrated that the electronic wiring is, in fact, less important than the ionic. We have constructed an experimental graph showing the dependence of electrode resistance on the particle size. The analysis has shown that the dependence follows almost exactly a square law, regardless of the quality of electronic wiring. Using modelling on a continuum level, we have demonstrated that in such a case the square law can only be observed if the ionic conductivity is much smaller than the electronic. Almost simultaneously, a group from the Max-Planck Institute in Stuttgart published measurements of ionic and electronic conductivities of lithium phosphate at high temperatures which were in conformity with our predictions (unfortunately, low-temperature conductivity measurements cannot be performed at the present level of methodology development).

It can be predicted that our findings will serve as important guidelines in future designing of nanoarchitectural features of battery cathodes. In particular, more focus will have to be given to further reduction of particle size and to providing more space around the particles for effi-



SLIKA 1:
Empirični zakon, ki povezuje elektrodno upornost in velikost aktivnih delcev ter shematska razlaga zakona.

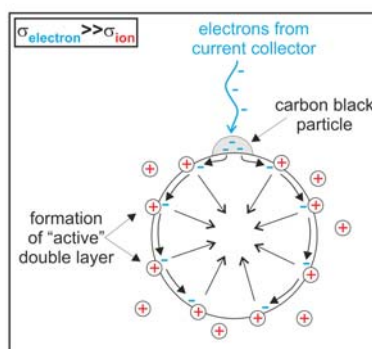
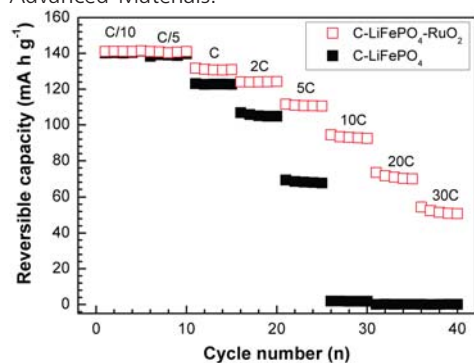


FIGURE 1:
Empirical law that correlates electrode resistance with active particle size in lithium batteries and a schematical explanation.

poskrbeti tudi za elektronsko ožičenje, vendar bo dovolj, da delce točkasto kontaktiramo s prevodnikom (homogeni ogljikovi filmi odslej ne bodo več primarnega pomena).

Izboljšava kinetike v katodnih materialih za litijeve baterije

Že v gornjem prispevku smo pojasnili, da je za delovanje sodobnih katodnih materialov za litijeve baterije material potrebno elektronsko in ionsko ožičiti. Za elektronsko ožičenje praktično vsi raziskovalci uporabljajo prevodne ogljikove materiale – zgoraj smo navedli primer nanometerskega ogljikovega filma. Iz nebatarijskih raziskav pa so že nekaj časa znani postopki priprave ožičenja poroznih materialov z rutenijevim oksidom, ki je za nekaj redov boljši elektronski prevodnik kot grafit. V sodelovanju z inštitutom Maxa Plancka v Stuttgartu smo po enem od teh postopkov ožičili naš porozni litijev fosfat, ki je sicer izvorno že deloma ožičen z ogljikovim materialom. Izkazalo se je, da dodatno ožičenje z rutenijevim oksidom izrazito izboljša kinetiko polnjenja-praznjenja tega materiala. Izboljšanje je najbolj očitno pri velikih tokovnih gostotah – izboljšani postopek tako omogoča, da material napolnimo hitreje kot v 1 minuti. Raziskavo smo objavili v prestižni reviji *Advanced Materials*.



SLIKA 2:

Schematski prikaz ožičenja katodnega materiala z rutenijevom oksidom (prirejeno iz članka, objavljenega v *Advanced Materials*)

cient access of electrolyte (ionic wiring). While the electronic wiring will still be important, it will not be considered crucial anymore; it will probably suffice to point contact individual particles with an electronic conductor.

Improvement of the kinetics of cathode materials for lithium batteries

As explained above, the new generation of high-capacity but low-conductivity cathodes for lithium batteries has to be appropriately electronically and ionically wired. For electronic wiring, researchers have almost exclusively used conductive carbons in various forms, for example, as nanometre-thick films mentioned above. In non-battery fields of research, however, other materials have been successfully used for wiring the interior of porous systems. An example is ruthenium oxide the conductivity of which exceeds the carbon conductivity by several orders of magnitude. In cooperation with Max-Planck Institute from Stuttgart we have used ruthenium oxide as an additional wiring material to the carbon material that forms in rather small quantities during preparation of a porous lithium phosphate. The electrochemical testing of such a »double-wired« material showed

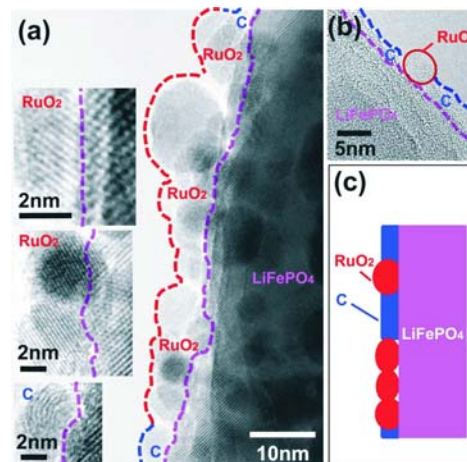


FIGURE 2:

Schematic presentation of wiring of a cathode material using ruthenium oxide (adopted from a paper published in *Advanced Materials*)

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Iskra TELA d.d., PE Baterije Zmaj, Šentvid pri Stični: optimizacija baterijskih elektrod;
- Krka d. d., Novo Mesto: raziskave tabletiranja izbranih učinkovin;
- Lek d.d., Ljubljana: priprava kompozitov s kontroliranim sproščanjem učinkovin;
- Predilnica Litija, partner v Centru odličnosti Nanoznanosti in nanotehnologije, ESRR, ukrep 1.1. in 1.4;
- Atotech Podnart, d.d., partner v Centru odličnosti Nanoznanosti in nanotehnologije, ESRR, ukrep 1.1. in 1.4.

MEDNARODNO SODELOVANJE

- ALISTORE, mreža odličnosti v 6. okvirnem programu EU;
- Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics (FP6-2004-NMP-NI-4) - NANO(BIOPHARMACEUTICS, Integrirani projekt (Ips) znotraj 6. evropskega okvirnega programa;
- APOLLON B, Advanced PEM Fuel Cells« (APOLLON-B), STREP EU project (do junija 2007).

POMEMBNI INSTRUMENTI IN OPREMA

- Vrščni 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).

a substantial improvement of the electrode kinetics if compared to the properties of carbon-wired phosphate. The improvement is especially remarkable at high current drains – the improved material allows charging of cathode in less than 1 minute. The work was published in *Advanced Materials*, a prestigious journal in the field of Materials Science.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Iskra TELA d.d., PE Baterije Zmaj, Šentvid pri Stični, Slovenia: optimisation of battery electrodes;
- Krka d.d., Ljubljana, Slovenia: tableting of selected drugs;
- Lek d.d., Ljubljana, Slovenia: composites with controlled release of drugs;
- Predilnica Litija, Slovenia, partner in Nanosciences and Nanotechnologies Centre of Excellence;
- Atotech Podnart, d.d., Slovenia, partner in Nanosciences and Nanotechnologies Centre of Excellence.

INTERNATIONAL COLLABORATION

- ALISTORE, 6th EU Framework Network of Excellence
- Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics (FP6-2004-NMP-NI-4) - NANO(BIOPHARMACEUTICS, Integrated project in the 6th EU Framework.
- APOLLON B, Advanced PEM Fuel Cells« (APOLLON-B), STREP EU project (until June 2007)

MAJOR EQUIPMENT

- Field-Emission Scanning Electron Microscope (Karl Zeiss Supra 35 VP, equipped with EDS (Oxford INCA 400)
- Systems for electrochemical, impedance, microimpedance and electrical measurements (EG&G Model 283, Solartron SI 1260, ECI 1286, FRA 1250, HP 4284 LCR meter, Karl Süss, Keithley 237)

IZOBRAŽEVANJE IN OBISKI

Doktorat:

- Dušan Strmčnik: Aktivna mesta za reakcije v PEM gorivnih celicah v modelnih in realnih sistemih; doktorska disertacija, mentor: doc. dr. Miran Gaberšček.

Mentorstva:

- Aljaž Godec: Vpliv prostorske restrikcije na nastanek in stabilnost polimorfnih in amorfni oblik; diplomska naloga, somentor: doc. dr. Miran Gaberšček;
- Uroš Maver: Nov hibridni kserogel silike za stabilizacijo in kontrolirano sproščanje učinkovin; diplomska naloga, somentor: dr. Marjan Bele.

Tuji raziskovalci na KI:

- Donato E. Conte je med marcem in septembrom 2007 v okviru Evropskega magistrskega študija pod vodstvom dr. R. Dominka v Laboratoriju L10 pripravil magistrsko delo. Magistrsko delo je uspešno zagovarjal v Franciji.

Raziskovalci KI v tujini:

- Robert Dominko, Université de Picardie, Amiens, Francija ter Max-Planck Institut, Stuttgart, Nemčija;
- Mirjana Küzma, Univerza Uppsala, Švedska;
- Janko Jamnik, Max-Planck Institut, Stuttgart, Nemčija;
- Miran Gaberšček, Univerza St. Andrews, Škotska.

Poletna šola: Računska kemija in litijeve ionske baterije

Pod okriljem Evropske mreže odličnosti ALISTORE je v obdobju med 16. in 20. julijem 2007 Laboratorij L10 organiziral poletno šolo z naslovom: Računska kemija in litijeve ionske baterije ("Computational Chemistry and Li-Ion Batteries"). Šola je potekala v veliki predavalnici Kemijskega inštituta. Program je bil organiziran tako, da od udeležencev ni zahteval posebnega predznanja. Obsegal je dokaj širok nabor znanj - od uvoda v kvantno mehaniko do praktične

- 2 Braun dry boxes (humidity < 1ppm, oxygen < 5ppm)

EDUCATION AND IMPORTANT VISITS

Ph. D. Thesis:

- Dušan Strmčnik: Active sites for PEM fuel cell reactions in model and real systems, ph.d. Dissertation. Mentor: Dr. Miran Gaberšček, Assist. Prof.

Mentorships:

- Aljaž Godec: The influence of space restriction on the formation and stability of polymorphic and amorphous forms (Diploma work). Comentor: Dr. Miran Gaberšček, Assist. Prof.
- Uroš Maver: Novel hybrid silica xerogels for stabilization and controlled release of drug, (Diploma work). Comentor: Dr. Marjan Bele.

Visiting researchers:

- From March to September 2007 Donato E. Conte successfully prepared a Master Thesis within the framework of European Masters. The experimental work was carried out in our Laboratory under the mentorship of Dr. Robert Dominko, while the Thesis was defended in France.

Visits of foreign Institutions

- Robert Dominko, Université de Picardie, Amiens, France and Max-Planck Institute, Stuttgart, Germany;
- Mirjana Küzma, Uppsala University, Sweden;
- Janko Jamnik, Max-Planck Institute, Stuttgart, Germany;
- Miran Gaberšček, University of St. Andrews, Scotland.

Summer School on "Computational Chemistry and Li-Ion Batteries"

From July 16th to 20th, 2007 the Laboratory organized an ALISTORE Theory Summer School (ATSS 2007) on "Computational Chemistry and Li-Ion Batteries". The school was held at the National Institute of Chemistry. The programme was organised such that no special pre-knowl-

uporabe izbranih računskih postopkov za obravnavo konkretnih baterijskih struktur. Naslovi učnih sklopov so bili naslednji:

- Osnove kvantne kemije
- Od molekul do trdne snovi
- Density Functional Theory (DFT)
- Spektroskopija in teorija
- Uporaba DFT pri študiju litijevih baterij

Predavatelji so bili: Marie-Liesse Doublet, Maria Elena Arroyo, Anton Kokalj, Pierre-Emmanuel Lippens in Michel Ménétrier. Šole se je udeležilo 20 študentov iz 6 evropskih držav.

edge was necessary. It was spanned from the introduction to quantum mechanics up to the consideration of specific examples from the real life of Li-batteries. The specific topics were the following:

- Basic notions of Quantum Chemistry
- From Molecules to Solids
- The Density Functional Theory (DFT)
- Spectroscopies and Theory
- Applications of Density Functional Theory (DFT) to Lithium battery

The lecturers were Marie-Liesse Doublet, Maria Elena Arroyo, Tone Kokalj, Pierre-Emmanuel Lippens and Michel Ménétrier. All the lectures are available on ALISTORE Website. There were more than 20 attendees from 6 European countries, all from ALISTORE-connected institutions.



SLIKA 3:
Skupinska fotografije udeležencev Poletne šole

FIGURE 3:
Group photography of participants of the Theory Summer School

L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation



VODJA / HEAD
prof. dr. Radovan Komel

RAZISKOVALCI / RESEARCHERS

dr. Gabrijela Ambrožič (LEK)
dr. Marija Anžur-Lasnik (LEK)
dr. Apolonija Bedina Zavec
Maja Capuder
dr. Vladimira Gaberc-Porekar
dr. Katja Galeša
dr. Simona Jevševar (LEK)
dr. Maja Kenig (LEK)
dr. Branka Korošec
dr. Nada Kraševc

Menči Kunstelj (LEK)
dr. Ana Lenassi Zupan
dr. Viktor Menart (KI/LEK)
dr. Mateja Novak Štagoj
Barbara Podobnik (LEK)
dr. Marjetka Podobnik
mag. Tatjana Preradov
mag. Vanja Smilović
mag. Irena Zore (LEK)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Urška Dermol
Petra Draškovič
Gorazd Hribar
Mateja Kusterle (LEK)
Ljerka Lah
Špela Peternel
Matjaž Vogelsang

TEHNIČNO OSEBJE / TECHNICAL STAFF

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

PRIPRAVNIKI / TRAINEES

Špela Jalen



PODROČJA DEJAVNOSTI

- Preučevanje metod za pridobivanje biofarmaceutikov - rekombinantnih citokinov ter njihova modifikacija
- Celična biologija kvasovke *S. cerevisiae*
- Biotehnologija nižjih evkariontov (nitaste glive in kvasovke)
- Preučevanje in kloniranje genov za pretvorbe steroidov pri nitastih glivah
- Strukturne raziskave biološko aktivnih molekul
- Funkcijska genomika

BIBLIOGRAFIJA

- 9 izvirmih znanstvenih člankov
- 1 poljudni članek
- 1 samostojni znanstveni sestavek v monografiji
- 1 intervju
- 1 objavljeni znanstveni prispevek na konferenci (vabljeni predavanje)
- 3 objavljeni znanstveni prispevki na konferencah

RESEARCH ACTIVITIES

- Investigation of approaches to biotechnological production of biopharmaceuticals - recombinant cytokines and their modification
- Cell biology of the yeast *Saccharomyces cerevisiae*
- Biotechnology of lower eukaryotes (filamentous fungi and yeasts)
- Study and cloning of steroid bioconverting genes in filamentous fungi
- Structural studies of biologically active molecules
- Functional genomics

BIBLIOGRAPHY

- 9 Original Scientific Articles
- 1 Popular Article
- 1 Independent Scientific Component Part in a Monograph
- 1 Interview
- 1 Published Scientific Conference Contribution (Invited Lecture)
- 3 Published Scientific Conference Contributions

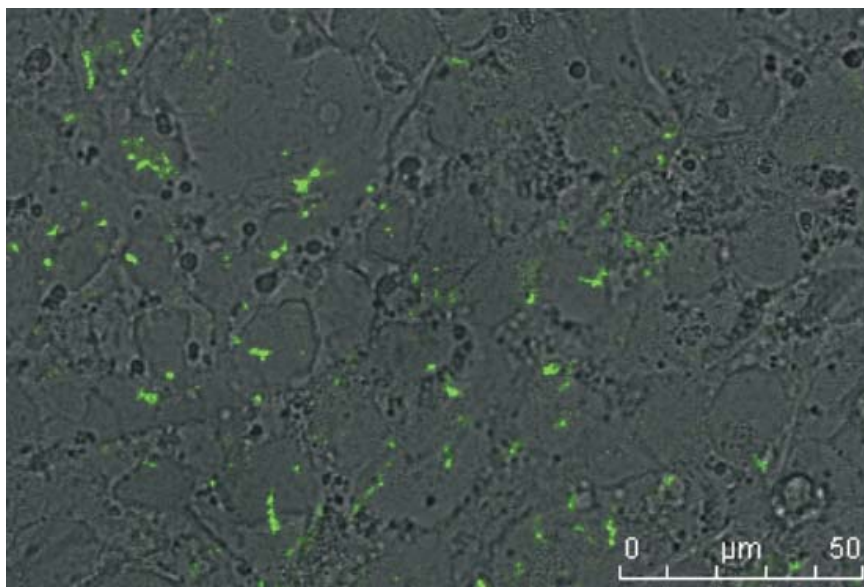
1	objavljeni strokovni prispevek na konferenci	1	Published Professional Conference Contribution
35	objavljenih povzetkov znanstvenih prispevkov na konferencah	35	Published Scientific Conference Contribution Abstracts
3	objavljeni povzetki strokovnih prispevkov na konferencah	3	Published Professional Conference Contribution Abstracts
1	patentna prijava	1	Patent Application
1	patent	1	Patent
1	prispevek na konferenci brez natisa	1	Unpublished Conference Contribution
3	vabljeni predavanja na konferencah brez natisa	3	Unpublished Invited Conference Lectures
3	doktorati	3	Doctoral Dissertations
2	uredništvi revij	2	Journal Editorships

GLAVNI DOSEŽKI V LETU 2007

V okviru evropskega projekta projekta »Nanoscale Functionalities for Targeted Drug Delivery of Biopharmaceutics« (»Nanobiopharmaceutics«), v katerem je Kemijski inštitut eden od partnerjev, smo pripravili v večjih količinah

MAIN ACHIEVEMENTS IN 2007

National Institute of Chemistry is one of the partners in the European FW6 project entitled »Nanoscale Functionalities for Targeted Drug Delivery of Biopharmaceutics« (»Nanobiopharmaceutics«). In the frame of this project 100 mg amounts of various tumor necrosis fac-



SLIKA 1:

Delci, pripravljani s samozdruževanjem TNF-alfa analoga LK-801, lokalizirani znotraj Caco-2 celic, ki služijo kot model za študij prehajanja intestinalnega epitelijskega (opazovano na konfokalnem mikroskopu). Protein, uporabljen za formiranje nanodelcev, je N-terminalno označen z Alexa Fluor 488. λ_{ex} : 488 nm; λ_{em} : 510-530 nm.

FIGURE 1:

TNF-alpha analogue LK-801 self-assembly nanoparticles localised inside Caco-2 cells, serving as a model for intestinal epithelium barrier (observed under confocal microscope). Proteins used for nanoparticles formation are N-terminally labeled with Alexa Fluor 488. λ_{ex} : 488 nm; λ_{em} : 510-530 nm.

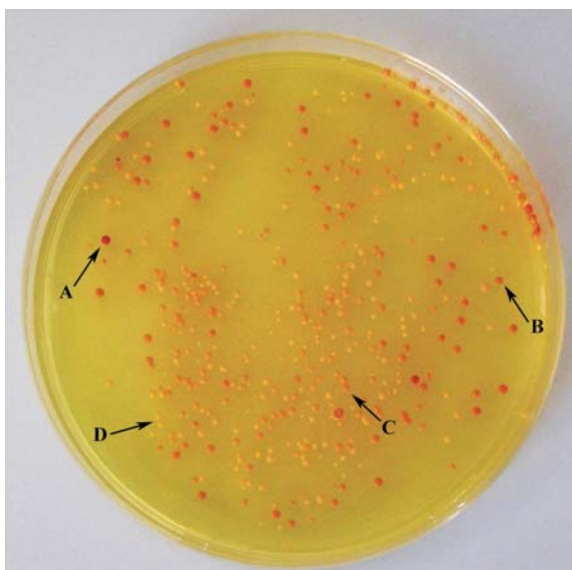
analoge faktorja tumorske nekroze alfa. Analogi so oblikovani tako, da vsebujejo regije, bogate s histidini, kar omogoča vezavo preko kovinskih ionov na podlagi koordinativnih vezi. To lastnost smo uporabili za kontrolirano nastajanje proteinskih nanodelcev ob dodatku biokompatibilnih kelatorskih molekul in za vezavo na različne tipe anorganskih delcev. Vse vrste delcev smo okarakterizirali glede na velikost in biološko aktivnost ter določili pogoje sproščanja posameznih proteinskih molekul.

Raziskave nastajanja »neklasičnih« inkluzijskih teles v sklopu biosinteze rekombinantnih proteinov smo razširili na različne proteine, saj je pojav tvorbe inkluzijskih teles z visokim deležem pravilno zvitega tarčnega proteina oziroma njegovega prekurzorja, ki ga je mogoče izolirati z blago ekstrakcijo v nenedenaturirajočih

tor alpha analogues containing histidine rich surface regions were prepared. Binding via coordinative mode enabled controlled formation of protein nanoparticles, as well as binding to various types of inorganic nanoparticles. The particles formed were characterized in respect of size and biological activity. Studies on stability of nanoparticles and controlled release of individual protein molecules were performed.

Formation of "non-classical" inclusion bodies containing a high amount of correctly folded target protein or its precursor that can be isolated by mild extraction under non-denaturing conditions is interesting not only from the scientific point of view but also for applications in biotechnology.

Therefore studies of »nonclassical« inclusion bodies (in the frame of research on biosynthe-



SLIKA 2:

Nova metoda za selekcijo visokoproduktivnih sevov kvasovke *Pichia pastoris* neposredno na plošči. Visokoproduktivne klone selekcioniramo vizuelno, odvisno od intenzitete rjave barve kolonij, ki je sorazmerna aktivnosti β -laktamaze (temno rjava, visoka aktivnost β -laktamaze; svetlo rjava, nizka aktivnost β -laktamaze). A – visoka aktivnost; B – srednja aktivnost; C – nizka aktivnost; D – brez aktivnosti.

FIGURE 2:

A new method for selecting high-producing yeast clones of *Pichia pastoris*. On-plate selection of transformants: high-producing clones are selected visually, based on the intensity of the brown color of the colonies that is proportional to the beta-lactamase activity (dark brown, high beta-lactamase activity; light brown, low beta-lactamase activity). A - high activity; B - medium activity; C - low activity; D - no activity.

pogojih, zanimiv ne le z znanstvenega stališča, ampak odpira tudi široke možnosti za aplikacijo v biotehnologiji.

V okviru projekta »Rekombinantno cepivo proti aviarni influenci« smo pripravili visoko-produktivne seve kvasovke *Pichia pastoris*, ki so primerni za biosintezo različnih oblik proteina hemaglutinin (HA) tip H5, ter nekatere oblike izolirali v obliki fluorescentnih nanodelcev. Poskusi na Veterinarski fakulteti so pokazali, da so tako pripravljene nanodelci sposobni sprožiti imunski odziv pri piščancih.

Raziskave v okviru ESRR iz delovnega paketa »Raziskave in biosinteza biofarmaceutikov«, ki so predvidevale razvoj celotne inovativne tehnologije za pridobivanje proteinskega biofarmaceutika A, smo v letu 2007 zaključili z uspešnim prenosom postopka v večje merilo, kar omogoča pridobivanje gramskih količin farmacevtskega proteina. Posamezne segmente tehnologije smo tudi patentno zaščitili. Vložene so bile mednarodne patentne prijave za razvoj visoko-produkcijskega seva, za postopek biosinteze in ekstrakcije brez denaturacije in renaturacije rekombinantnega proteina, dve prijavi za dva različna postopka separacije in dve prijavi za formulacije končnega proteina. Rezultati raziskave diferencialnega izražanja genov (s poudarkom na genih, ki kodirajo citokrome P450 nitaste glive *Cochliobolus lunatus*) po dodatku progesterona so pokazali, da steroid v glivi izzove globalni stresni odgovor. Hkrati z določanjem zaporedij velikemu številu klonov cDNA pa je naša raziskava ponudila tudi vpogled v doslej še neznan genom nemo-delnega organizma. Nadalje smo v sklopu preučevanja citokromov P450 izbrane glive z uporabo PCR v realnem času kvantitativno ovrednotili relativno raven izražanja genov za dve reduktazi citokromov P450 (CPR) in pet citokromov P450 po dodatku progesterona. Oba gena za CPR smo izrazili v bakteriji *E. coli* in funkcionalnost proteinskih produktov potrdili spektrofotometrično. V teku so funkcijske raziskave obeh reduktaz v rekonstitucijskih sistemih z različnimi citokromi P450 iz glive *C.*

sis of recombinant proteins) were extended to different proteins.

Research on "Recombinant vaccine against avian influenza" resulted in some high-producing strains of *Pichia pastoris* that express various forms of hemagglutinin. The selected proteins were isolated in the form of fluorescent nanoparticles and assessed for eliciting immune response in chickens (experiments performed at Veterinary Faculty, University of Ljubljana). The main objective of the »Research on biosynthesis of biopharmaceuticals« in the frame of ESRR project was to develop an innovative technology for production of an interesting pharmaceutical protein. In 2007 the studies were concluded by a successful transfer of the process to a larger scale, enabling production of gram quantities of the pharmaceutical protein. For several technology segments international patent applications were filed covering the development of the high-producing strain, extraction of the correctly folded protein from inclusion bodies, two different separation procedures and two types of pharmaceutical formulations.

The results of a differential gene expression study, with emphasis on genes coding for cytochromes P450, upon progesterone treatment of the filamentous fungus *Cochliobolus lunatus* suggest that progesterone induces a global adaptive stress response in the organism. An additional inevitable consequence of the large-scale sequencing of cDNA clones, valuable insight into the genome of this non-model organism was obtained. Furthering our research on cytochromes P450 from *C. lunatus* we performed a quantitative expression analysis of two cytochrome P450 reductase (CPR) genes and five cytochrome P450 genes using real-time PCR. Both CPR genes were expressed in the *E. coli* expression system and functional activities of protein products were confirmed using a spectrophotometric assay. Functional studies of CPRs in reconstitution systems with different cytochromes P450 are in process.

Within structural studies of inositol polyphos-

lunatus.

V okviru projekta strukturnih raziskav inozitol polifosfatnih kinaz smo analizirali produkte encimske katalize treh izooblik sesalske inozitol heksakisfosfatne kinaze (IP6K). Vse tri proteine smo izrazili v *E. coli* in jih tudi ustrezno očistili. Produkta encimske reakcije IP6K (inozitol polifosfate (PP-IP), ki vsebujejo energetsko bogate fosfo-anhidridne vezi) smo pripravili *in vitro* v merilu, primernem za strukturne študije z masno spektrometrijo in nuklearno magnetno resonanco. Razvili smo postopke za čiščenje strukturno raznolikih PP-IP, ki jih sintetizira IP6K, ter postopke za analizo z omenjenimi strukturnimi metodami. Pokazali smo, da vse tri izooblike IP6K sintetizirajo enak izbor produktov, ki vsebujejo tako difosfatne in/ali trifosfatne skupine, vezane na inozitolni obroč. Produkti encimske katalize encima IP6K so biološko pomembne molekule, ki igrajo vlogo pri uravnavanju rekombinacije DNA, ohranjanju dolžine telomer, odzivu na stres, vezikularnem transportu, kemotaksiji, apoptozi ter fosforilaciji proteinov. Zato naše raziskave polifosforiliranih inozitolov predstavljajo pomemben doprinos k razumevanju mehanističnega ozadja teh bioloških procesov.

V letu 2007 smo objavili prvo kristalno strukturo katalitične domene encima Rv0805 iz *Mycobacterium tuberculosis* in s tem tudi prvo strukturo proteina iz razreda III fosfodiesteraz cikličnih nukleotidov. Rv0805 je do sedaj edina znana fosfodiesteraza tega razreda v genomu patogene bakterije *M. tuberculosis* (Shenoy et al., 2007). S proučevanjem te mikrobakterijske in njej sorodnih fosfodiesteraz tudi v drugih bakterijah, pa tudi evkariontskih organizmih, želimo razložiti mehanizem njihovega delovanja, ravno tako pa tudi način evlucijskega prilagajanja strukturno podobnih aktivnih mest na različne vloge v različnih organizmih, posebno še v patoloških stanjih.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Laboratorij združuje raziskovalce KI in Lek

phate kinases, we have analyzed the products of the enzymatic reaction catalyzed by three isoforms of the mammalian inositol hexakisphosphate kinase (IP6K). All three proteins were expressed in *E. coli* and purified for further studies. Products of the enzymatic reaction by IP6K (inositol polyphosphates (PP-IP) containing energetically rich phospho-anhydride bonds) were prepared *in vitro* in large scale, and were further used in structural studies by mass spectrometry and nuclear magnetic resonance. Protocols have been developed for the purification of various PP-IPs synthesized by IP6K as well as for the structural analysis of these molecules. We have shown that all three IP6K isoforms synthesize the same assortment of PP-IPs, which contain di- and/or tri-phosphate groups attached to the inositol ring. The products of IP6K catalysis are biologically important molecules, playing role in regulation of DNA recombination, telomere length maintenance, response to stress, vesicular trafficking, chemotaxis, apoptosis and modification of proteins by phosphorylation. Therefore our structural studies on polyphosphorylated inositols represent an important contribution to understanding of basic mechanisms behind these biological processes.

In 2007 we published the first crystal structure of the catalytic domain of the Rv0805 enzyme from *Mycobacterium tuberculosis* (Shenoy et al., 2007), which is also the first known structure of the protein belonging to the class III of the cyclic nucleotide phosphodiesterases. Rv0805 is thus far the only known phosphodiesterase of this class in the genome of the pathogenic bacterium *M. tuberculosis*. Our studies on this mycobacterial enzyme as well as on other related enzymes in eukaryotes, are important for understanding the evolutionary adaptation seen in this class of enzymes, with similar architecture of active sites but perhaps tuned to different functions. Especially if their roles are associated to pathogenic states.

d.d., Biofarmacevtika, tako da gre za mešano skupino, ki že vrsto let deluje na skupnih raziskovalnih projektih;

- vodenje oz. koordiniranje Centra odličnosti ESRR (Evropski strukturni skladi za regionalni razvoj) »Biotehnologija s farmacijo«, ki združuje 18 partnerjev – univerzitetnih ustanov, raziskovalnih inštitutov, zdravstvenih ustanov, S&M podjetij in slovenske farmacevtske industrije. L11 vodi raziskovalno-razvojni projekt CO RRP2 »Načrtovanje, pridobivanje in karakterizacija biofarmaceutikov«.

MEDNARODNO SODELOVANJE

- 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; 2006 - 2009);
- MIRG-6-CT-2005-014882: EC Marie Curie International Reintegration Grant "Structural Studies of Inositol poly-Phosphate Kinases" (M. Podobnik; 2005 - 2007);
- ICGEB CSA (International Centre for Genetic Engineering and Biotechnology): R. Komel - član Znanstvenega sveta ICGEB (CSA - Council of Scientific Advisers; drugi mandat 2007 - 2009);
- EC mreža odličnosti NANOFUN-POLY (V. Menart, V. Gaberc-Porekar - članstvo v mreži odličnosti; 2004 - 2007);
- Indian Institute of Science, Bangalore, Indija: sodelovanje s prof. Sandhya Visweswariah na projektu "Strukturne študije cAMP-fosfodiesteraze iz *M.tuberculosis*" (M. Podobnik);
- Johns Hopkins University Medical School, Baltimore, USA: sodelovanje z dr. Rashina Bhandari iz laboratorija prof. Solomona Snyderja na projektu "Strukturne raziskave inozitol polifosfatnih kinaz" (M. Podobnik);
- Medical Research Council Laboratory for Molecular Cell Biology and Cell Biology Unit, University College London, Gower Street,

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Laboratory L11 represents a research group composed of researchers from the National Institute of Chemistry (NIC) and the Pharmaceutical Company LEK, d.d., Biopharmaceuticals, Slovenia, which work together on selected research projects.
- Heading and coordinating the Centre of Excellence (CoE) "Biotechnology with Pharmacy" at European Structural Funds for Regional Development (ESRR), associating 18 partners – from university institutions, public research institutes, medical & health care institutions, S&M enterprises and Slovenian pharmaceutical industry. Laboratory L11 is coordinating CoE R&D project 2 "Design, production and characterization of biopharmaceuticals".

INTERNATIONAL COLLABORATION

- FW6-2004-NMP-NI-4; IP 026723-2 NANO-BIOPHARMACEUTICALS: Integrated FW6 Project "Nanotechnology-Based Targeted Drug Delivery" (V. Gaberc-Porekar, V. Menart – project partnership; 2005/06 - 2008/09)
- MIRG-6-CT-2005-014882: EC Marie Curie International Reintegration Grant "Structural Studies of Inositol poly-Phosphate Kinases" (M. Podobnik; 2005 - 2007)
- ICGEB CSA (International Centre for Genetic Engineering and Biotechnology): R. Komel – CSA Member (CSA – ICGEB Council of Scientific Advisers; 2nd mandate, 2007 - 2009)
- EC Network of Excellence NANOFUN-POLY (V. Menart, V. Gaberc-Porekar – membership; 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.

London WC1E 6BT, UK. Sodelovanje z dr. Adolfom Saiardijem (M. Podobnik).

POMEMBNI INŠTRUMENTI IN OPREMA

- Laboratorij za gensko tehnologijo
- Laboratorij za izolacijo, čiščenje in karakterizacijo (rekombinantnih) proteinov
- Laboratorij za celične kulture
- Mikrobiološki laboratorij
- Laboratorij z bioreaktorji
- Laboratorij za nanobiotehnologijo
- Kriobanka

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

- Pretočni citometer z možnostjo sortiranja celic (Beckman Coulter);
- Konfokalni mikroskop Leica TCS SP5 (Leica Microsystems, z laserskimi linijami 405, 458, 476, 488, 514, 543, 633);
- Fluorescenčni mikroskop (Zeiss) s sistemom za slikanje;
- Stereo mikroskop (Nikon);
- Fluorimeter (PTI);
- 2 UV/VIS spektrofotometra (Agilent, Hewlett-Packard);
- Chirascan CD Spectrometer (Applied Photo-physics, konzorcij);
- Dynamic Light Scattering Detector (DynaPro);
- ProExpress Imaging System za denzitometrično obdelavo (Perkin Elmer);
- Isothermal Titration Calorimeter (MicroCal, konzorcij);
- 5 preparativnih sistemov za kromatografske separacije proteinov (Amersham Biosciences, Knauer);
- 2 analitska HPLC sistema (Waters, Knauer);
- 2 računalniško vodena laboratorijska bioreaktorja (Applikon);
- 3 sistemi za pripravo Milli-Q vode (Millipore);

Rashina Bhandari from the laboratory of Prof. Solomon Snyder on the "Structural studies of inositol poly-phosphate kinases" project (M. Podobnik).

- Medical Research Council Laboratory for Molecular Cell Biology and Cell Biology Unit, University College London, Gower Street, London WC1E 6BT, UK. Collaboration with Dr. Adolf Saiardi (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
- Laboratory for nanobiototechnology
- Cryobank

Laboratories are equipped with modern instruments for the realization of the above mentioned projects. This is the list of more significant instruments:

- Flow cytometer with cell sorter (Beckman Coulter)
- Confocal microscope Leica TCS SP5 (Leica Microsystems, with laser lines 405, 458, 476, 488, 514, 543, 633)
- Fluorescence microscope with CD camera (Zeiss)
- Stereo microscope (Nikon)
- Fluorimeter (PTI)
- 2 UV/VIS spectrophotometers (Agilent, Hewlett-Packard)
- Chirascan CD Spectrometer (Applied Photo-physics, consortium)
- Dynamic Light Scattering Detector (DynaPro)
- ProExpress Imaging System for densitometric analysis (Perkin Elmer)
- Isothermal Titration Calorimeter (MicroCal)
- 5 preparative HPLC systems for protein separations (Amersham Biosciences, Knauer)

- hladilne kapacitete +4°C, -20°C in -70°C;
- 4 stresalniki;
- sklop aparatov za pomnoževanje in sekvenčno analizo DNA;
- system za dokumentacijo gelov (Chemi Doc, BIO-RAD);
- ultracentrifuga (Beckman L7-55).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Doktorati:

- Maja Kenig (mentor: doc. dr. Viktor Menart);
- Simona Jevševar (mentor: doc. dr. Viktor Menart);
- *Irena Zupanič Pajnič (mentor: prof. dr. Radovan Komel, na Medicinski fakulteti Univerze v Ljubljani);
- *Alja Videtič (mentor: prof. dr. Radovan Komel, na Medicinski fakulteti Univerze v Ljubljani).

Diplomska dela:

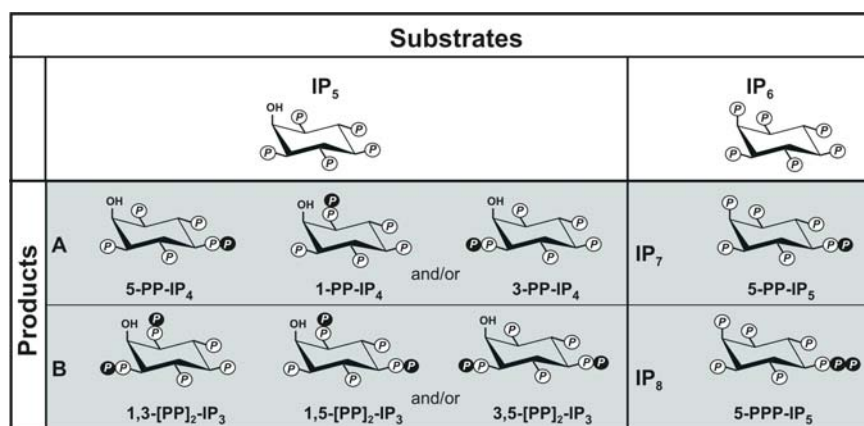
- Jana Herman (mentorica: dr. Maja Kenig) – tudi Prešernova nagrada Fakultete za

- 2 Analytical HPLC systems (Waters, Knauer)
- 2 computer assisted laboratory bio-reactors (Applikon)
- 3 systems for Milli-Q water (Millipore)
- Cooling and freezing capacities (+4°C, -20°C and -70°C)
- Gel documentation system (Chemi-Doc, BIORAD)
- Shakers and Incubators
- Set of instruments for PCR and DNA sequence analysis
- ultracentrifuge (Beckman L7-55)

EDUCATION AND IMPORTANT VISITS

PhD Theses:

- Maja Kenig (supervisor: Dr. Viktor Menart, Assist. Prof.)
- Simona Jevševar (supervisor: Dr. Viktor Menart, Assist. Prof.)
- *Irena Zupanič Pajnič (supervisor: Prof. Dr. Radovan Komel, at Medical Faculty, University of Ljubljana)



SLIKA 3:

Inozitol polifosfati, ki jih sintetizira IP6K iz dveh naravnih substratov, inozitol pentakisfosfata (IP₅) in inozitol heksakisfosfata (IP₆). Sivo ozadje: strukture produktov, ki smo jih določili v naši skupini (IP₇, IP₈, A, B) z uporabo masne spektrometrije in NMR. Fosfatne skupine, ki jih na substrata doda IP6K, so ozančene s črnimi krogi.

FIGURE 3:

Inositol polyphosphates synthesized by IP6K from two natural substrates, inositol pentakisphosphate (IP₅) and inositol hexakisphosphate (IP₆). Gray background: structures of products determined in our group (IP₇, IP₈, A, B) using mass spectrometry and NMR. Phosphate groups added by IP6K to the substrates are marked with black balls.

- farmacijo Univerze v Ljubljani;
- *Rok Kopinč (mentor: prof. dr. Radovan Komel, na Medicinski fakulteti Univerze v Ljubljani);
 - *Tina Tinkara Peternej (mentor: prof. dr. Radovan Komel, na Medicinski fakulteti Univerze v Ljubljani);
 - *Barbara Zajec (mentor: prof. dr. Radovan Komel, na Medicinski fakulteti Univerze v Ljubljani);
 - *Nina Kočevar (mentor: prof. dr. Radovan Komel, na Medicinski fakulteti Univerze v Ljubljani).

Obiski:

- Dr. Carlo R. Bruschi, Dimitri Nikitin (ICGEB, Trst, Italija): sodelovanje na področju pretočne citometrije;
- Dr. Kurt Wagemann (DECHEMA): sodelovanje v okviru FW6 EC projekta NANOBIPHARMACEUTICS;
- Prof. dr. Sandhya S. Visweswariah (Indian Institute of Science, Bangalore, Indija): sodelovanje v okviru raziskav na fosfodiesterah.

- *Alja Videtič (supervisor: Prof. Dr. Radovan Komel, at Medical Faculty, University of Ljubljana)

Diploma works:

- Jana Herman (supervisor: Dr. Maja Kenig) – as well receiving Prešeren award for graduation from the Faculty of Pharmacy, University of Ljubljana)
- *Rok Kopinč (supervisor: Prof. Dr. Radovan Komel, at Medical Faculty, University of Ljubljana)
- *Tina Tinkara Peternej (supervisor: Prof. Dr. Radovan Komel, at Medical Faculty, University of Ljubljana)
- *Barbara Zajec (supervisor: Prof. Dr. Radovan Komel, at at Medical Faculty, University of Ljubljana)
- *Nina Kočevar (supervisor: Prof. Dr. Radovan Komel, at Medical Faculty, University of Ljubljana)

Visits:

- Dr. Carlo R. Bruschi, Dimitri Nikitin (ICGEB, Trieste, Italy): collaboration in the field of flow cytometry
- Dr. Kurt Wagemann (DECHEMA): collaboration in the frame of FW6 EC project NANOBIPHARMACEUTICS
- Prof. Dr. Sandhya S. Visweswariah (Indian Institute of Science, Bangalore, India): collaboration in the research of phosphodiesterases



IN MEMORIAM

doc. dr. Viktor Menart

V začetku februarja 2007 nas je nepričakovano in mnogo prezgodaj zapustil naš dolgoletni sodelavec, doc. dr. Viktor Menart.

Viktor Menart se je rodil 30.5.1951 na Kalcah pri Logatcu. Po študiju kemije na Fakulteti za naravoslovje in tehnologijo (FNT) v Ljubljani, ki ga je zaključil z diplomom na področju organske kemije pri prof. dr. Branku Stanovniku, je podiplomski študij nadaljeval pri prof. dr. Borutu Plesničarju, kasneje pa je bil asistent pri prof. dr. Cvetu Klofutarju.

Njegovo poklicno pot je začrtal prihod v farmacevtsko družbo Lek, kjer se je zaposlil leta 1983 kot vodja analitske službe v enoti Kontrola. Osebno zanimanje za področje genskega inženirstva ga je leta 1989 privedlo na mesto vodje oddelka Biotehnologija v enoti Razvoj in raziskave, kjer se je vključil v projekt Peptidi, ki pomeni začetek razvoja biofarmacevtikov za humano uporabo v Leku. Raziskave rekombinantnih proteinov so se začele na Kemijskem inštitutu (KI), kjer se je ob koncu osemdesetih let izoblikovala mešana skupina raziskovalcev iz Leka in KI ter so se opremili laboratoriji za gensko inženirstvo. Viktor Menart je aktivno sodeloval pri uvajanju metod genskega in proteinskega inženirstva. Začetne raziskave so bile usmerjene v preučevanje pridobivanja tedaj

IN MEMORIAM

doc. dr. Viktor Menart

Our colleague of many years Dr. Viktor Menart, Assist. Prof. unexpectedly and much too early passed away in the beginning of February 2007.

He was born in Kalce near Logatec on May 30, 1951. After finishing the study of chemistry at the Faculty of Natural Sciences and Technology in Ljubljana with a diploma of organic chemistry (under the mentorship of Prof. Dr. Branko Stanovnik), he continued his post graduation studies under the guidance of Prof. Dr. Borut Plesničar and later as assistant of Prof. Dr. Cvetu Klofutar.

His professional career was strongly marked by his transition to the Pharmaceutical Company Lek in 1983, where he became the head of Analytics in the Control department. Personal interest in genetic engineering lead him to the heading position in the department of Biotechnology within the Research & Development. The Peptide project of that time was the starting point for further development of biopharmaceuticals in Lek. Research of recombinant proteins started at the National Institute of Chemistry (NIC), where in the late eighties a mixed group of researchers from NIC and Lek was formed and the laboratories for genetic engineering were set up. Viktor Menart

zelo perspektivne farmacevtsko uporabne molekule, dejavnika tumorske nekroze alfa (TNF-alfa), kmalu pa so se razširile na nove analoge TNF-alfa in preučevanje povezav med njihovo strukturo in funkcijo. To je bilo področje, na katerem je Viktor Menart lahko razvijal svojo kreativnost in uresničeval svoje inovativne ideje. V tem času je nastala večina rezultatov, ki jih je leta 2000 zaokrožil v doktorski disertaciji z naslovom "Novi analogi faktorja tumorske nekroze (TNF-alfa) - možnosti uporabe v molekularni biologiji ter pri zdravljenju in diagnostiki rakastih bolezni", ki jo je opravil pod mentorskim vodstvom prof. dr. Franca Gubenška.

Čeprav je bil Viktorju Menartu že od leta 1989 Kemijski inštitut njegov drugi dom, kjer je potekalo njegovo raziskovalno delo, ki je bilo bistvo njegovega delovanja in življenja, se je šele konec leta 2000 formalno dopolnilno zaposlil na Kemijskem inštitutu, v Laboratoriju za biosintezo in biotransformacijo. To mu je omogočalo bolj odprto in neposredno navezovanje stikov z raziskovalci po svetu, prijavljanje raziskovalnih projektov, mentorstva mladih raziskovalcev in utrjevanje sodelovanja med družbo Lek in raziskovalnimi ustanovami v Sloveniji ter drugod po svetu. Prizadeval si je za čim tesnejše sodelovanje med industrijo in raziskovalnim inštitutom, jedro katerega je bila že omenjena mešana skupina, sestavljena iz raziskovalcev Leka in raziskovalcev s Kemijskega inštituta. Sadovi zelo uspešnega dolgoletnega sodelovanja se kažejo v številnih znanstvenih publikacijah, mednarodnih patentih in patentnih prijavih z inovativnimi rešitvami, ki so omogočile razširitev raziskovalnega področja na številne farmacevtske proteine in prehod v razvojne in strateške Lekove projekte.

Najbolj odmeven in tudi za Lek najpomembnejši je bil razvoj tehnologije rekombinantnega filgrastima. V letu 2003 je dr. Viktor Menart za "Projekt Filgrastim (Razvoj produkcijskega seva, tehnologije biosinteze in postopka izolacije filgrastima)" skupaj z mag. Simono Jevševar iz Farmacevtske družbe Lek d.d. ter dr. Vladko

took an active part in introduction of genetic and protein engineering methods. Initial studies were connected with biosynthesis and production of tumour necrosis factor alpha (TNF-alpha), a very prospective pharmaceutically relevant molecule of that time, and broadened to design and development of numerous novel TNF-alpha analogues and their structure – relationship studies. This was the research area where Viktor Menart could employ his creativity and fulfil innovative ideas. Results from that time were collected in his doctoral thesis entitled "Novel analogues of tumour necrosis factor alpha (TNF-alpha) – use in molecular biology, in cancer treatment and diagnostics", which was prepared under the mentorship of Prof. Dr. Franc Gubenšek.

Although since 1989 the National Institute of Chemistry was Dr. Viktor Menart's second home, where his research, an essential part of his activities and life took place, he became a formal member of NIC only in 2000. He took a part-time researcher position in the Department of biosynthesis and biotransformation. As a member of the Institute he could communicate more openly with researchers from different institutions and countries, apply for research projects and guide young researchers. This new role also contributed to consolidation of connections between company Lek and research institutions in Slovenia and abroad. Strong collaboration was established between the industry and the research institute, especially within the previously mentioned mixed group of researchers from Lek and NIC. Successful long-term collaboration has resulted in numerous scientific publications and international patents and patent applications. On the basis of innovative solutions the initial studies expanded to various pharmaceutically relevant proteins and grew to important developmental and strategic projects of Lek.

Most sounded and for Lek most important was the technology development of recombinant filgrastim. In 2003 Dr. Viktor Menart received, together with Dr. Simona Jevševar (Pharma-

Gaberc Porekar s Kemijskega inštituta prejel zlato priznanje Gospodarske zbornice Slovenije za inovacije. Istega leta je za svoje delo prejel tudi Lekovo plaketo dela. Njegovo delo velja za pionirsko na področju uvajanja rekombinantne tehnologije v Leku.

Dr. Viktor Menart je bil vrhunski strokovnjak s širokim znanjem, človek z drugačnimi idejami in jasno začrtanimi cilji. Svoje znanje in pogled v prihodnost je prenašal na mlade raziskovalce in v njih spodbujal veselje do raziskovanja in do ustvarjalnega, bolj inovativnega razmišljanja. Spominjali se ga bomo kot človeka, ki mu je raziskovanje pomenilo več kot delo in dolžnost, človeka, za katerega je bilo raziskovanje vsebina njegovega življenja, njegovo veselje, ustvarjalnost in poslanstvo.

Dr. Vladka Gaberc Porekar (NIC), a golden award of the Chamber of Economy of Slovenia for the innovations on Filgrastim (Development of production strain, technology of biosynthesis and isolation procedure). In the same year Dr. Viktor Menart was awarded the Lek medal for his pioneering work in the introduction of recombinant technology in the company.

Dr. Viktor Menart was a top-expert with broad knowledge, a man of different ideas and clearly set goals. He disseminated his knowledge and his views to young researchers, stimulating their wish to explore and to think in a creative and innovative way. In or memory he will remain a man, for whom the research was more than work and duty, for whom the research was the substance of his life, his joy, creativity and mission.

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

Matevž Avbelj
Tanja Bagar
Lorena Butinar
Iva Hafner Bratkovič
Monika Ciglič
Jernej Gašperšič
Karolina Ivičak
Boštjan Japelj
Nina Klemenčič
Tina Šolar
Martina Mohorčič
Blaž Nemeč
Gabrijela Panter
Nina Pirher
Nuša Resman
Mireille Treeby Premuš
Andreja Šmerc
Aleksandra Usenik
Jožica Vašl
Mojca Zelnikar
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, ki imajo potencialno uporabnost (predvsem biotehnoško, medicinsko in farmacevtsko). Pri tem uporabljamo moderne metode znanosti o življenju, kot so biokemija, molekularna in celična biologija, mikrobiologija, biofizika in strukturna biologija ter bioinformatika.

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

RESEARCH ACTIVITIES

Activities of the Department of Biotechnology primarily include research of biochemical processes, such as biomolecular recognition and signal transduction within cells, which have potential application relevant for health (biotechnological, medicinal, pharmaceutical). We use a wide range of modern methods of life sciences including biochemistry, molecular and cell biology, microbiology, biophysics, structural biology and bioinformatics.

Main research topics are molecular mechanisms of innate immunity, conformational diseases and structure of amyloids, as well as the mechanisms and design of antimicrobial agents. We are particularly interested in the mechanisms of recognition and biological activity at the molecular level, especially molecular patterns characteristic for pathogenic microorganisms (PAMP), therefore we use instrumental methods with high resolution and sensitivity, such as nuclear magnetic resonance (NMR) and fluorescent spectroscopy. Our research includes physiology studies of microorganisms producing enzymes, organic acids, antibiotics and other pharmaceuticals, as well as recombinant proteins.

BIBLIOGRAFIJA

- 17 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 1 kratki znanstveni prispevek
- 1 strokovni članek
- 1 samostojni znanstveni sestavek v monografiji
- 4 intervjuji
- 1 drugi članek ali sestavek
- 3 objavljeni znanstveni prispevki na konferencah
- 19 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 3 patenti
- 3 predavanja na tujih univerzah
- 1 prispevek na konferenci brez natisa
- 3 vabljeni predavanja na konferencah brez natisa
- 6 diplom
- 3 doktorati

GLAVNI DOSEŽKI V LETU 2007

Velik del raziskav v laboratoriju je potekal na področju imunskega prepoznavanja bakterijskih infekcij. Te raziskave omogočajo razumevanje delovanja imunskega sistema kot obrambe pred okužbo z mikroorganizmi in kot zaščito pred nevarnostjo, kar se pogosto kaže v obliki kroničnih vnetij. Pri teh procesih pomembno vlogo igrajo receptorji družine Toll, med katerimi raziskujemo predvsem receptorje TLR3 in TLR4 skupaj z njegovim koreceptorjem MD-2. V sodelovanju z raziskovalci iz Univerze v Iowi (ZDA) smo analizirali vpliv naravnih polimorfizmov MD-2 na vezavo LPS in signalizacijo. Ugotovili smo, da polimorfna oblika G56R zniža odzivnost celic na LPS, sam MD-2 pa sploh ni sposoben vezati LPS ampak je potrebno, da nastopa v obliki kompleksa z izvenselično domeno TLR4. To odkritje, katerega poročilo je v tisku v reviji *Journal of Immunology*, ima velik pomen predvsem za odzivnost na celice, ki same ne proizvajajo MD-2 (npr. epiteljske celice v dihalih, ki so konstantno izpostavljene visokim koncentracijam endotoksina) in so odvisne od MD-2, ki ga proizvajajo druge celice.

BIBLIOGRAPHY

- 17 Original Scientific Articles
- 1 Review Article
- 1 Short Scientific Article
- 1 Professional Article
- 1 Independent Scientific Chapter in Monography
- 4 Interviews
- 1 Other Article
- 3 Published Scientific Conference Contributions
- 19 Published Scientific Conference Contribution Abstracts
- 3 Patents
- 3 Invited Lectures at Foreign Universities
- 1 Unpublished Conference Contribution
- 3 Unpublished Invited Conference Lectures
- 6 Undergraduate Theses
- 3 PhD Theses

MAIN ACHIEVEMENTS IN 2007

An important part of our research was devoted to the immunological recognition of bacterial infections. This research enables comprehension of the immune system activity in the function of protection and defence against infection with microorganisms what often appears in the form of chronic inflammation. In these processes Toll-like receptors play an important role. Among them we are mostly studying TLR3 and TLR4 with its co-receptor MD-2. In cooperation with researchers from the University of Iowa (USA) we have analysed the effect of natural polymorphisms of human MD-2 on LPS binding and cell signalization. We found that the polymorphic form of the G56R impaired the cellular response to LPS, while MD-2 variant itself was not able to bind LPS except when it was in complex with the TLR4 ectodomain. This discovery is most relevant for the responsiveness of cells that themselves do not produce MD-2 (e.g. epithelial cells in respiratory tract, which are constantly exposed to high concentrations of endotoxin) and are dependent on MD-2 produced by other cells. The report of discovery is in press in the *Journal of Immunology*.

V okviru raziskav nevtralizacije bakterijskega endotoksina in antimikrobnih peptidov smo določili prostorske strukture več (lipo)peptidov v okolju membranskih mimetikov. Delo je bilo nadaljevanje sicer zaključenega EU projekta ANEPID. Del rezultatov projekta smo prijavili kot mednarodni patent, ter v znanstvenih publikacijah v revijah kot je J.Am.Chem.Soc. in Expert Opinion in Investigational Drugs.

Na področju konformacijskih bolezni, predvsem prionskih bolezni, smo raziskovali molekularni mehanizem pretvorbe prionskega proteina in potencialno uporabo tako dobljenih spoznanj za preprečevanje pretvorbe in hitrejšo ter bolj občutljivo diagnostiko infektivnosti. S pomočjo vezave spojine naravnega izvora, kurkumina, smo ugotovili možnost inhibicije pretvorbe preko vezave na vmesno strukturo na prehodu med nativno ter fibrilizirano obliko. V tej obliki je porušena nativna terciarna struktura proteina, vendar protein ostaja večinoma v obliki alfa vijačnice. Vezan kurkumin se nahaja v asimetričnem okolju, katerega lahko opredelimo s pomočjo cirkularnega dihroizma. To je prvi primer identifikacije vezave inhibitorja na prehodno stanje in pomeni nov pristop k iskanju zdravil proti prionskim boleznim. Rezultate smo objavili v članku v reviji Journal of Neurochemistry. Na osnovi analize prostorske strukture prionskega proteina in biokemijskih podatkov smo pripravili mutante PrP, od katerih so nekatere odporne na pretvorbo, druge pa se pretvorijo hitreje, kar ima lahko pomen za zaščito in pripravo hitrejšega in bolj občutljivega testa za detekcijo infektivnosti biološkega materiala.

Na področju študija regulacije primarnega metabolizma pri različnih organizmih, smo nadaljevali z raziskavami 6-fosfofrukto-1-kinaze (PFK1). Ugotovili smo, da se ta ključni regulatorni encim glikolize lahko posttranslacijsko spremeni. To povzroči nastanek aktivnega kratkega fragmenta, ki je odporen na inhibicijo povratne zveze, nekateri aktivatorji pa pospešijo njegovo delovanje v večji meri kot je to primer pri nativnem encimu. Nastanek kratkega

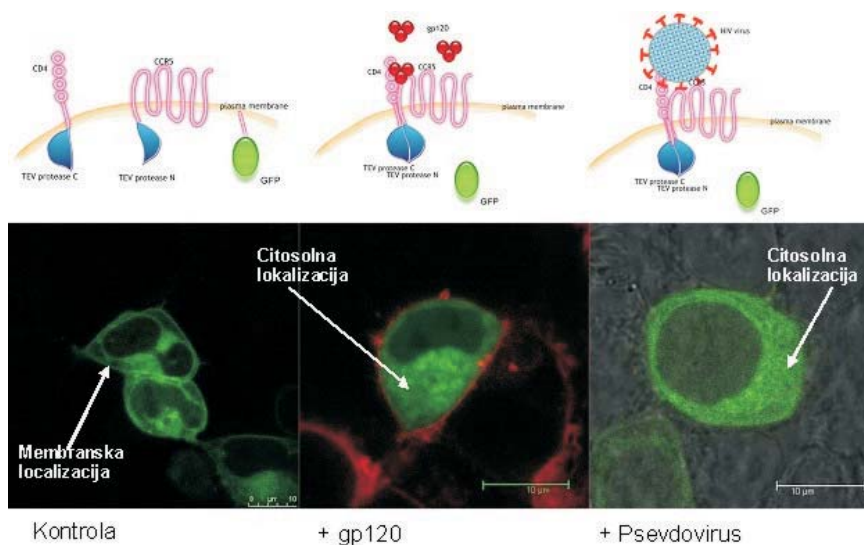
Within the research on neutralization of bacterial endotoxin and antimicrobial peptides we determined spatial structures of several (lipo)peptides in the environment of membrane mimetics. The research was a continuation of the finished EU project ANEPID. Part of the results was included in the international patent application, and some in scientific publications in journals such as J. Am. Chem. Soc. and Expert Opinion in Investigational Drugs.

Within the research of conformational diseases, in the first place prion diseases, we studied molecular mechanism of transformation of prion protein and potential application for prevention of pathological transformation of prion protein and for faster and more sensitive diagnosis of infectivity. Through binding of a compound of natural origin, curcumin, we discovered the possibility to inhibit the transformation by means of binding to the structural intermediate between the native and fibrillized form of PrP. In this form the defined native tertiary structure of the protein is disrupted, however, the protein remains mostly in the form of alpha helix. Bound curcumin is located in an asymmetrical environment which could be inferred by means of induced circular dichroism effect. This is the first report of identification of the inhibitor binding to the intermediate state and it represents a new approach to drug discovery against prion diseases. Our results were published in the Journal of Neurochemistry. Based on the analysis of spatial structure of prion protein and biochemical data we prepared mutants PrP, some of which were resistant to conversion while the others transform faster which can be important for health and on the other hand for preparation of a quicker and more sensitive test for detection of infectivity of biological material.

By studying regulation of primary metabolism in different organisms, we continued the research on 6-phosphofructo-1-kinase (PFK1). We found that this key regulatory glycolytic enzyme can undergo posttranslational modifi-

fragmenta v končni fazi povzroči povečan, nekontroliran pretok metabolitov preko glikolize, kar pripelje do neuravnoteženja katabolnih in anabolnih procesov v celici. Spontani posttranslacijski modifikaciji PFK1 se lahko izognemo z vnosom kratkega mutiranega *pfkA* gena v celice, ki v transformantah omogoča neposredno sintezo aktivnega kratkega fragmenta. Za uporabo intelektualnih pravic sta pokazali interes dve tuji biotehnoški družbi, ki nameravata gen preizkusiti. Paralelno smo poskusili dokazati, da do podobne posttranslacijske modifikacije PFK1 pride tudi ob transformaciji normalnih sesalčnih celic v neoplastične, rakaste celice. Močan metabolni pretok preko glikolize ter nastajanje laktata je namreč značilnost večine metastaznih celic. Z Western analizo smo dokali,

This leads to the formation of an active short fragment, which is resistant to feed-back inhibition, while some activators increase its activity to a larger extent than in the case of the native enzyme. The formation of the short fragment finally causes an increased, uncontrolled metabolite flux through glycolysis what leads to unbalanced catabolic and anabolic processes in the cell. A spontaneous post-translational modification can be avoided by introduction of a mutated truncated *pfkA* gene into the cell, which enables a direct synthesis of the active fragment in the transformants. Two biotechnological companies showed interest for the use of the gene which was protected by a PCT patent application.



SLIKA 1:
 Prikaz umetne naprave za zaznavanje virusne infekcije na človeških celicah. Zgornja slika prikazuje shemo aktivacije TEV proteaze ob vezavi virusnih proteinov na človeške celice, kjer smo namesto T7 RNA polimeraze uporabili reporterski zeleni fluorescenčni protein (GFP). Dodatek virusnega proteina gp120 ali posevdovirusa je povzročil premik proteina z membrane v citosol.

FIGURE 1:
 Schematic presentation of the HIV detection device and its experimental confirmation. The upper figure illustrates the mechanism of activation of split TEV protease by binding of viral components to human cells where we used reporter green fluorescent protein (GFP) instead of T7 RNA polymerase. Addition of viral protein gp120 or of pseudovirus caused translocation of the protein from the membrane into the cytosol.

da pri transformiranih celičnih linijah ni prisoten nativni PFK1 encim, s specifičnimi protitelesi pa zaznamo krajše fragmente. Pri kontrolnih celicah, normalnih limfocitih, smo detektirali le nativni protein. Posttraslacijsko modifikacijo sesalčjega PFK1 encima smo uspeli dokazati tudi pod *in vitro* pogoji.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Lek, d.d., Ljubljana: raziskave na področju biotehnologije ter razvoju novih zdravil;
- BIA Separations d.o.o, Ljubljana;
- Kimi d.o.o., Trzin.

MEDNARODNO SODELOVANJE

v mednarodnih projektih:

- Dva evropska projekta v okviru 6. okvirnega programa: Eurofungbase in TSEUR;
- bilateralno sodelovanje s Hrvaško, Argenino, ZDA in Indijo;
- COST projekt D25: "Applied biocatalysis: Stereoslective and environmentally-friendly reactions catalysed by enzymes".

pogodbe s podjetji v tujini:

- DSM Food Specialists, Nizozemska;
- Novozyme, Danska;
- Jungbunzlauer, Švica.

neformalno sodelovanje z drugimi znanstvenimi ustanovami po svetu:

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

POMEMBNI INŠTRUMENTI IN OPREMA

- Pretočni citometer s sorterjem EPICS® ALTRA™, Beckman Coulter
- Laserski konfokalni fluorescenčni mikroskop Leica DMI3000B
- CD spektrometer Chirascan, Applied Photo-physics

In parallel, we tried to prove that similar posttranslational modification occurred also in transformation of normal mammalian cells into neoplastic, cancer cells. High metabolic flux through glycolysis and formation of lactate is namely characteristic of most metastatic cells. By using Western blot we proved that in the transformed cell lines the native PFK1 enzyme was not present, while with the specific antibodies short fragments were detected. When healthy lymphocytes have been taken as a control, only the native protein was detected. The posttranslational modification of the mammalian PFK1 enzyme was shown also under the *in vitro* conditions.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Lek, d.d., Ljubljana, Slovenia: research in the filed of biotechnology and drug development;
- BIA Separations d.o.o, Ljubljana, Slovenia;
- Kimi d.o.o., Trzin, Slovenia.

INTERNATIONAL COLLABORATION

international projects:

- Two EU projects in the FW6: Eurofungbase and TSEUR
- Bilateral collaboration with Croatia, USA, India and Argentina
- COST project D25: "Applied biocatalysis: Stereoslective and environmentally-friendly reactions catalysed by enzymes"

contracts with companies from abroad:

- DSM Food Specialists, The Netherlands
- Novozyme, Danmark
- Jungbunzlauer, Switzerland

informal collaboration with other academic institutions in the world:

- University of Strathclyde, Glasgow, United Kingdom
- University of Edinburgh, Edinburgh, United Kingdom

- UV/VIS spektrometer, Perkin Elmer Lambda 25
- Fluorescenčni luminometer, Perkin Elmer LS-55
- Luminometer/fluorimeter za mikrotitrne plošče z injektorjem, Mitras
- Grafična postaja Silicon Graphics Fuel s programsko opremo za NMR, molekularno modeliranje in SAR
- Bioreaktor Infors
- HPLC in drugi kromatografski instrumenti
- Sistem za 2D elektroforezo s programsko opremo (Melanie)
- Laboratorij za delo z mikroorganizmi
- Laboratorij za delo s celičnimi kulturami
- Technische Universität Graz, Austria
- Universidad de Navarra, Pamplona, Spain
- Indian Institute of Science, Bangalore, India

MAJOR EQUIPMENT

- Flow cytometer with cell sorter EPICS® ALTRA™, Beckman Coulter
- Laser confocal fluorescent microscope Leica DMI3000B
- CD spectrometer Chirascan, Applied Photophysics
- UV/VIS spektrometer, Perkin Elmer Lambda 25
- Fluorescentluminometer, Perkin Elmer LS-55
- Luminometer/fluorimeter for microtiter plates with injector, Mitras
- Graphical workstation Silicon Graphics Fuel with software for NMR, molecular modeling and SAR analysis
- Bioreactor Infors
- HPLC and other chromatographical instruments
- System for 2D electrophoresis with software for data evaluation (Melanie)
- Laboratory for microbiology
- Laboratory for cell culture

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Pet sodelavcev L12 je habilitiranih za sodelovanje pri do- in podiplomskem študiju Univerze v Ljubljani;
- v letu 2007 je bilo narejenih 6 diplomskih del in 3 doktorska dela;
- gostovanje podiplomskega študenta Gorana Mikluševića iz Hrvaške in podiplomske študentke Kirsten Altenbach iz Velike Britanije.

DOSEŽEK ODMEVEN V MEDIJIH

Raziskovalci Laboratorija za biotehnologijo so tudi v letu 2007 organizirali študentsko raziskovalno ekipo za pripravo raziskovalnega projekta s področja sintezne biologije iGEM (international Genetically Engineered Machines). Na izboru članov ekipe smo izbrali sedem študentov biokemije, mikrobiologije in biotehnologije. Pri izvedbi projekta je v vlogi mentorjev sodelovalo pet raziskovalcev Laboratorija za biotehnologijo Kemijskega inštituta, ter doc. Marko Dolinar s FKKT, pri delu pa so pomagali tudi drugi člani laboratorija. Za cilj projekta smo si letos izbrali pripravo obrambe človeških celic proti virusu HIV-1, tako da le-ta ne bi bila odvisna od virusnih mutacij. Ta cilj smo dosegli tako, da smo zaznavanje virusa izvedli preko uporabe

EDUCATION AND IMPORTANT VISITS

- Five members of the Department L12 participate as lecturers or demonstrators at the under- and postgraduate level at the University of Ljubljana;
- Six BSc theses and three PhD theses have been defended in 2007;
- research visits of PhD students Goran Miklušević from Croatia and Kirsten Altenbach from United Kingdom.

ACHIEVEMENT NOTED IN THE MEDIA

Researchers of the Department of Biotechnology mentored the student research team for

funkcije virusa, neodvisno od posameznega aminokislinskega zaporedja, ki ga virus lahko spreminja z mutacijami in s pomočjo katerih postane odporen na zdravila in se izogne imunskemu sistemu. Za ta namen smo izkoristili vezavo virusa na celico kjer se veže na receptorja CD4 in CCR5, kar lahko zaznamo s tvorbo dimera preko rekonstitucije cepljenega ubikvitina ali TEV proteaze. Ta dogodek preko proteolitske cepitve sprosti z membrane T7 RNA polimerazo. Ta RNA polimeraza vodi do prepisovanja izbranih efektorskih proteinov, ki celici omogočijo obrambo pred virusom. Na osnovi podobnega principa smo zaznali aktivnost proteaze virusa HIV, ki mora cepiti določeno aminokislinsko zaporedje virusnega proproteina. To razpoznavno zaporedje smo vstavili kot povezovalni peptid med membranskim sidrom in T7 RNA polimerazo in ob prisotnosti aktivne virusne proteaze se podobno kot prej sproži prepisovanje efektorskih proteinov, ki bodisi povzročijo propad okuženih celic in tako preprečijo razširitev infekcije ali povečajo sposobnost sosednjih celic za obrambo pred virusom. Vse naštetje funkcije smo dokazali eksperimentalno z uporabo virusnih proteinov in nenevarnega psevdovirusa. Tekmovanja se je udeležilo 56 ekip z vsega sveta, med katerimi so bile tudi najuglednejše univerze kot so ameriške Harvard, Stanford, Berkeley, Princeton, MIT... evropske univerze Cambridge, ETH, Pariz, Freiburg... ter azijske Bangalore, Tokio ter letos prvič tudi štiri najboljše kitajske univerze. Lansko leto je na omenjenem tekmovanju slovenska ekipa dosegla izjemen uspeh z osvojitvijo prvega mesta s projektom zdravljenja sepse, letos pa je nova ekipa ljubljanskih študentov ponovila odličen uspeh z uvrstitvijo med šest finalistov, osvojitvijo zlate medalje ter prvega mesta med projekti s področja zdravja in medicine. Člani ekipe so bili študenti Katja Kolar, Anja Korenčič, Rok Gaber, Andrej Ondračka, Peter Cimermančič, Saša Jereb, Marko Bitenc, mentorji pa prof. Roman Jerala, doc. Marko Dolinar, dr. Mateja Manček

the preparation of a research project in the field of synthetic biology iGEM (international Genetically Engineered Machines). Based on the proposed projects we have selected students of biochemistry, microbiology and biotechnology. Five researchers from the Department of Biotechnology at the National Institute of Chemistry were involved as mentors in addition to the mentor from the Faculty of Chemistry and Chemical Technology, University of Ljubljana. Other members of the Department also contributed to the success of the experimental work. The objective of this year's project was to prepare the defence of human cells against HIV-1 virus that would be insensitive to viral mutations. This objective was achieved in such a way that the viral detection was achieved based on the viral function independently of particular amino acid sequence which virus can change and becomes resistant to drugs or avoids the immune system. First utilized viral function was viral attachment to human cells where it binds to the receptors CD4 and CCR5. CD4-CCR5 heterodimer can be detected through the reconstitution of the split ubiquitin or TEV protease from C-terminal fusions of segments of ubiquitin or TEV protease attached to each of the co-receptors. Reconstitution of those reporters triggers the release of T7 RNA polymerase from the membrane via proteolytic cleavage. This RNA polymerase is targeted into the nucleus and leads to the transcription of the effector proteins that enable the defence of the cells against the virus. Based on the similar principle we detected the activity of the HIV protease that cleaves the defined amino acid sequence of the viral proprotein. We introduced this peptide sequence motif as the linker peptide between the membrane anchor and T7 RNA polymerase and proteolytic activity of the viral protease, similarly as above, triggered transcription of effector proteins that either caused the destruction of the infected cells and in such a way prevented further spread of infection or increased the capability of the neighbouring cells for defence against the virus. All of the listed functions were confirmed experimentally

Keber, dr. Mojca Benčina, Gabriela Panter in Karolina Ivičak. Informacija o projektu je dostopna na : <http://parts.mit.edu/igem07/index.php/Ljubljana>

Uspeh je bil deležen velike pozornosti medijev in je prispeval k zavesti o pomenu in sposobnostih slovenske znanosti in izobraževanja. Mentorji so prejeli nagrado Prometej znanosti za znanstveno komuniciranje, ki jo podeljuje Slovenska znanstvena fundacija ter Sokratovo odličje za visokošolsko didaktiko.

using viral proteins and the non-hazardous pseudovirus.

At the competition 56 teams from all over the world participated at the jamboree at MIT, among them there were the most prominent universities such as Harvard, Stanford, Berkeley, Princeton, MIT... from USA, Cambridge, ETH, Paris, Freiburg, ...from Europe, and Asian teams from Bangalore, Tokyo, and for the first time also four top Chinese universities. Last year, in the same competition, Slovenian team achieved an outstanding success by winning the first place with the project on synthetic biology approach towards treatment of sepsis and in 2007 a new team of students repeated the success by qualifying among the six finalist teams and by winning the gold medal and first place among the projects in the field of health and medicine. Team members were the following students: Katja Kolar, Anja Korenčič, Rok Gaber, Andrej Ondračka, Peter Cimermančič, Saša Jereb, Marko Bitenc, mentors were prof. Roman Jerala, asst. prof. Marko Dolinar, Dr. Mateja Manček Keber, Dr. Mojca Benčina, Gabriela Panter and Karolina Ivičak. Information on the project is available on the web: <http://parts.mit.edu/igem07/index.php/Ljubljana>

The success attracted a great attention of the media and contributed to the awareness about the importance and capabilities of Slovenian science and education. The mentors obtained the Prometheus Scientific Award for scientific communication granted by Slovenian Science Foundation, and Socrates Award for high education didactics.

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 Hočevnar
dr. Albin Pintar

**MLADI RAZISKOVALCI /
YOUNG RESEARCHERS**

Petar Djinović
David Perko (od / from 01. 10.)

TEHNIČNO OSEBJE / TECHNICAL STAFF

Urška Kaučič
Saška Javornik (od / from 16. 07.)



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 in Pd monometalnih katalizatorjev, uporabljenih v integriranem procesu za denitrifikacijo podtalnice;

RESEARCH ACTIVITIES

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

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

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

BIBLIOGRAFIJA

- 5 izvirnih znanstvenih člankov
- 1 pregledni znanstveni članek
- 1 samostojni znanstveni sestavek v monografiji
- 1 intervju
- 7 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 prispevek na konferenci brez natisa
- 1 elaborat, predštudija, študija
- 2 diplomi
- 1 doktorat
- 3 uredništva revij

GLAVNI DOSEŽKI V LETU 2007

- V okviru projekta APOLLON-B (6. OP EU) smo skupaj s kolegi iz Forschungszentrum Karlsruhe (FZK ITC-CPV) sintetizirali PtCu/CeO₂/C elektrokatalizator za katodno reakcijo redukcije kisika in anodno reakcijo oksidacije vodika v prisotnosti ogljikovega monoksida za nizkotemperaturne PEM gorivne celice. Skupaj s kolegi iz Argonne National Laboratory (ANL, Chicago, ZDA) smo določili specifično aktivnost katalizatorja v reakciji redukcije kisika in v reakciji oksidacije ogljikovega monoksida. Specifična aktivnost katalizatorja je glede na aktivno površino v

BIBLIOGRAPHY

- 5 Original Scientific Articles
- 1 Review Article
- 1 Independent Scientific Component Part in a Monograph
- 1 Interview
- 7 Published Scientific Conference Contribution Abstracts
- 1 Unpublished Conference Contribution
- 1 Treatise, Preliminary Study, Study
- 2 Undergraduate Theses
- 1 Doctoral Dissertation
- 3 Journal Editorships

IMPORTANT ACHIEVEMENTS IN 2007

- The PtCu/CeO₂/C electro-catalyst for the cathodic reduction of oxygen and the anodic oxidation of hydrogen in the presence of carbon monoxide for low-temperature PEM fuel cells was synthesized, together with Forschungszentrum Karlsruhe (FZK ITC-CPV) in the framework of APOLLON-B (6. OP EU) project. Textural characteristics and specific activities of the catalyst for oxygen reduction and carbon monoxide oxidation were determined, together with Argonne National Laboratory

prvi reakciji primerljiva z aktivnostjo Pt katalizatorja (Pt whiskers), ki ga je razvil koncern 3M (ZDA), v drugi reakciji pa je 16-krat aktivnejši od primerjalnega industrijskega katalizatorja firme E-Tek (Degussa). Rezultate je predstavil koordinator projekta na »Fuel Cells Review Days« Evropske tehnološke platforme za vodik in gorivne celice, 10. in 11. oktobra 2007 v Bruslju.

- Objavili smo samostojno poglavje v knjigi (S. Hočevar) »Renewable Resources and Renewable Energy: A global Challenge« (M. Graziani in P. Fornasiero, ur.), CRC Taylor & Francis, Boca Raton, FL, USA, 2007. [COBISS.SI-ID 3638042]
- Z uporabo dveh ločenih katalitskih reaktorjev s strnjenim slojem, napolnjenih s Pd-Cu oziroma Pd katalizatorjem, smo modificirali procesno shemo integriranega procesa za

(ANL, Chicago, USA). Specific activity of the catalyst in the first reaction is comparable with the activity of Pt catalyst (Pt whiskers), which was developed by the 3M (USA). Specific activity of the catalyst in second reaction is 16-times higher than the activity of benchmark industrial catalyst produced by E-Tek (Degussa). The coordinator of the project presented these results at the »Fuel Cells Review Days« meeting of European technology platform for hydrogen and fuel cells (EU HFP) on October 10-11th, 2007 in Brussels.

- S. Hočevar published chapter entitled »Hydrogen Production and Cleaning from Renewable Feedstock« in the book »Renewable Resources and Renewable Energy: A global Challenge« (Eds.: M. Graziani in P. Fornasiero), CRC Taylor & Francis, Boca Raton, FL, USA, 2007, 40 pp. [COBISS.SI-ID 3638042].



SLIKA:

Računalniško vodeni sistem za določevanje teksturalnih in adsorpcijskih lastnosti katalizatorjev in trdnih materialov (Micromeritics, model ASAP 2020 MP/C).

FIGURE:

Computer-controlled system for determination of textural and adsorption properties of catalysts and solid materials (Micromeritics, model ASAP 2020 MP/C).

odstranjevanje presežnih množin nitratnega iona iz pitne vode, s čimer se je drastično zmanjšala produkcija amonijevega iona kot stranskega produkta reakcije. [COBISS.SI-ID 3800090]

- Z različnimi tehnikami smo sintetizirali nanostrukturne $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-y}$ katalizatorje, preučevali pogoje sinteze na njihovo strukturo in morfologijo ter določili kvantitativne strukturno-aktivnostne odvisnosti v procesu sinteze vodnega plina (water gas shift reaction, WGSR), vodenem v pulzno obratujočem reaktorju. [COBISS.SI-ID 3647258]

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Z Ministrstvom za obrambo RS (MORS) smo sklenili pogodbo za izvedbo projekta s področja vodikovih tehnologij in gorivnih celic (števil. pog. 631-48/2007-77), pri kateri Laboratorij za katalizo in reakcijsko inženirstvo na Kemijskem inštitutu nastopa kot edini izvajalec (nosilec projekta dr. Gorazd Berčič).
- Z Ministrstvom za obrambo RS (MORS) smo sklenili pogodbo za izvedbo projekta s področja vodikovih tehnologij in gorivnih celic (števil. pog. 631-48/2007-78), pri kateri Laboratorij za katalizo in reakcijsko inženirstvo na Kemijskem inštitutu nastopa kot soizvajalec skupaj z Inštitutom »Jožef Stefan« in podjetjem HIPOT-RR raziskave in razvoj tehnologij in sistemov, d.o.o. (nosilec na Kl dr. Stanko Hočevar).

MEDNARODNO SODELOVANJE

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

- The process scheme of the integrated process for the removal of excess nitrate ions from potable water was modified by introducing two separate fixed bed catalytic reactors filled with Pd-Cu and Pd catalyst, respectively. Consequently, the formation of ammonium ion as a side-product was drastically lowered [COBISS.SI-ID 3800090].
- Nanostructured $\text{Cu}_x\text{Ce}_{1-x}\text{O}_{2-y}$ catalysts were synthesized using diverse techniques. The influence of synthesis parameters on their structure and morphology were studied, catalytic activities in water gas shift were determined with pulse microreactor and the structure-activity relationship were evaluated [COBISS.SI-ID 3647258].

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- The work was performed under contract with MoD RS (MORS) in the field of hydrogen and fuel cells (CT 631-48/2007-77, PI: Dr. Gorazd Berčič). The Laboratory of Catalysis and Chemical Reaction Engineering from National Institute of Chemistry is the only contractor for this project.
- The work was performed under contract with MoD RS (MORS) in the field of hydrogen and fuel cells (CT 631-48/2007-78, PI: Dr. Stanko Hočevar), in which the Laboratory of Catalysis and Chemical Reaction Engineering from National Institute of Chemistry is in partnership with Institute »Jožef Stefan« and company HIPOT-R&D.

INTERNATIONAL COLLABORATION

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

POMEMBNI INSTRUMENTI 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 opremljenih s sistemi za nadzor in zajemanje podatkov;
- 600 W sistem za testiranje gorivnih celic z računalniškim vodenjem (HP VEE OneLab);
- LabMax-ReactIR 1000 mešalni šaržni reaktor s sistemom za IR analizo reakcije v realnem času (Mettler Toledo);
- računalniško vodeni sistem za določevanje teksturalnih in adsorpcijskih lastnosti katalizatorjev in trdnih materialov (Micromeritics, model ASAP 2020);
- avtomatizirani sistem za karakterizacijo heterogenih katalizatorjev (Micromeritics, model Autochem II 2920);
- masni spektrometer (Pfeiffer Vacuum, model ThermoStar);
- računalniško vodeni, kontinuirni reaktorski sistem »Microactivity Reference« za študij dvo- in trifaznih katalitskih reakcij pri temperaturah do 750 stopinj Celzija in tlakih do 100 bar (PID Eng&Tech, Španija).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Doktorska disertacija:

- L. Zevnik: Karakterizacija s plinom ekspandiranih tekočin z akustično metodo; mentor: prof. dr. Janez Levec.

Diplomski deli:

- T. Nastran: Stacionarni model nizkotemperaturne gorivne celice s protonsko izmenjalno membrano; delovni mentor dr. Stanko Hočevar, mentor prof. dr. Janez Levec;
- D. Perko: Model membranskega reaktorja; mentor prof. dr. Janez Levec.

MAJOR EQUIPMENT

- HPLC + ChemStation (HP)
- several GCs with TCD and FID detector (HP)
- TOC analyzers in liquid and solid samples (Tekmar/Dohrmann)
- several batch CST, trickle-bed and fixed-bed laboratory reactors with data acquisition and control units
- 600 W fuel cell test station with HP VEE OneLab software-based data acquisition and control unit
- LabMax-ReactIR 1000 reactor and real-time reaction analysis system (Mettler Toledo)
- Automated system for heterogeneous catalysts characterization (Micromeritics, model Autochem II 2920)
- Mass spectrometer (Pfeiffer Vacuum, model ThermoStar)
- Computerized continuous-flow reactor system »Microactivity Reference« for studies of two- and three-phase catalytic reactions at temperatures up to 750 degrees C and pressures up to 100 bar (PID Eng&Tech, Spain)

EDUCATION AND IMPORTANT VISITS

Doctoral dissertation:

- L. Zevnik: Characterization of gas-expanded liquids with acoustic method; Supervisor: Prof. Dr. Janez Levec.

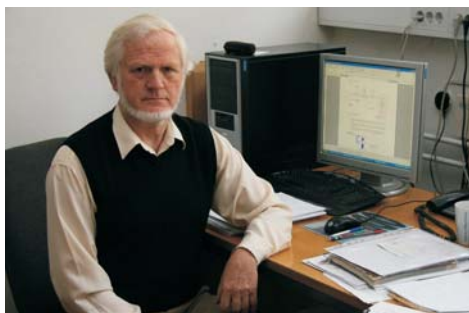
Undergraduate theses:

- T. Nastran: Stationary model of low-temperature PEMFC; Supervisors: Dr. Stanko Hočevar and Prof. Dr. Janez Levec;
- D. Perko: Membrane reactor model; Supervisor: Prof. Dr. Janez 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



PODROČJA DEJAVNOSTI

- Raziskave in razvoj procesov za proizvodnjo novih izdelkov, sodobnih separacijskih tehnik, modeliranje in optimiranje delovanja kritičnih procesnih elementov in naprav; odpravljanje ozkih grl procesov; izdelava tehnoloških podlag za nove ali inovirane procese; povečevanje novih proizvodnih postopkov iz laboratorijskega v pilotno in poindustrijsko merilo, izvajanje pilotnih poskusov, materialno-energetsko bilanciranje in modeliranje procesov.
- Merjenje izbranih fizikalno-kemijskih lastnosti čistih snovi, mešanic in materialov; modeliranje termodinamskih ravnotežij večfaznih oz. večkomponentnih sistemov v širšem obsegu termodinamskih pogojev PTC (tekoč-tekoče, tekoče-parno, tekoče-trdno) za potrebe načrtovanja teh operacij in naprav; razvoj materialov z veliko površino in kontrolirano dinamiko raztapljanja v specifičnih bioloških pogojih.
- Razvoj in integracija preventivnih ukrepov varstva okolja v industrijske procese; razvoj in uvajanje čistih tehnologij v industrijsko

RESEARCH ACTIVITIES

- Process research and development
- Research and development of new products and their production processes, development of scale-up methods for physical-chemical processes and their application in process development, process debottlenecking, process simulation and optimization, process-integrated environmental protection.
 - Measurement of thermodynamic properties (e.g. L-V, L-L and L-S equilibria) of various industrially important multicomponent mixtures in broad range of thermodynamic conditions PTC and their modelling by means of advanced statistical methods; microparticle formation of defined release properties.
 - Contribution of a monograph chapter on R&D in solubility problems of complex solid-liquid mixtures: effect of various physical-chemical properties of a solute on properties of saturated solution and final products, on process flowsheet and control diagram. Many typical industrial case problems and solutions are given.

prakso kot temelja trajnostnega industrijskega razvoja; adaptacija obstoječih procesov zahtevam BAT tehnologij po direktivi IPPC oz. izdelava ocen skladnosti z BAT; izdelava analiz življenjskega cikla izdelkov/storitev (paket GABI-4).

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

Ekspertize in svetovanje

- Izdelava in revizija poročil o vplivih proizvodnih in drugih procesov na okolje (pooblastilo MOP);
- izdelava načrtov za gospodarjenje z odpadki in ocen odpadkov (pooblastilo MOP);
- razvoj in izvajanje regeneracije čistih laboratorijskih in procesnih topil (dovoljenje MOP);
- nadzor načrtovanja in delovanja elementov za civilno zaščito (pooblastilo MO).

BIBLIOGRAFIJA

- 1 izvorni znanstveni članek
- 1 strokovni članek
- 1 samostojni znanstveni sestavek v monografiji
- 1 objavljeni znanstveni prispevek na konferenci
- 1 objavljeni strokovni prispevek na konferenci
- 1 objavljeni povzetek znanstvenega prispevka na konferenci
- 6 elaboratov, predštudij, študij
- 2 izvedenski mnenji, arbitražni odločbi
- 1 diploma
- 1 magisterij
- 2 uredništvu revij

GLAVNI DOSEŽKI V LETU 2007

- Izvajanje integriranega EU projekta BIOCOUP v okviru FP6-2004-Energy 3 z naslovom: »Co-

- Contribution of thermodynamic analysis to a deodoration study of vegetable oil, as a final step in its production process, by using alternative statistical thermodynamic models for prediction of phase equilibria.
- Integration of pollution prevention and environmental protection measures in new or existing industrial/infrastructural processes, development of reclamation processes for recyclable components from various waste process streams.
- Development and implementation of methods and procedures for identification, classification and characterization of hazardous wastes; research and development of pretreatment processes for difficult effluents and hazardous wastes in order to minimize their hazardness potential.
- National inventories and balances of critical environmental contaminants, wastes and emissions; life cycle assessment, identification and modelling of transport routes of selected contaminants in the environment, elaboration of environmental action programmes.
- Development of sustainable industrial processes, assessment of large industrial and environmental protection plants with respect to BAT-requirements, according to IPPC directive and BREF documents.

Expertise, consulting and service

- Environmental impact assessment studies; life cycle analysis (upon authorisation);
- waste management plans and waste assessment reports (upon authorisation);
- small scale production of specialty chemicals, reclamation of extra-pure laboratory solvents from waste mixtures, neutralization of hazardous laboratory chemicals (upon permission).

BIBLIOGRAPHY

- 1 Original Scientific Article
- 1 Professional Article

- processing of upgraded bio-liquids in standard refinery units« (sprejet v financiranje od leta 2006 dalje); posredovanje rezultatov na več srečanjih.
- Izradnja visokotlačne celice za merjenje faznih ravnotežij v okviru sodelovanja s firmo Bayer Technology Services, Leverkusen na področju visokotlačne in analitične tehnologije za določitev termodinamskih lastnosti materialov in sodelovanja z Univerzo Erlangen na področju tvorbe mikrodelcev v farmacevtske namene z uporabo SCF-GAS tehnike ter študija sproščanja zdravilnih učinkovin.
 - Poglavje v knjigi, ki opisuje razvoj in aplikacije topnosti (sistem trdno-tekoče). Prispevek obravnava pomen topnosti oziroma fizikalno kemijskih lastnosti pri načrtovanju procesov, saj kvaliteta teh lastnosti močno vpliva na kvaliteto končnega produkta. Fizikalno-kemijske lastnosti igrajo pomembno vlogo tudi pri modeliranju regulacijskih struktur. Poglavje je problemsko zasnovano, saj so predstavljeni aktualni problemi, ki izhajajo iz industrijske prakse.
 - Sodelovanje pri študiji optimizacije procesa deodorizacije, kot končne stopnje rafinacije jedilnega olja, z ustrezno izbranim modelom za popis termodinamskega ravnotežja tekočina-para obravnavanega večkomponentnega sistema.
 - Dogradnja državnega informacijskega sistema za področje odpadkov in izdelava nacionalnih bilanc in trendov komunalnih, nenevarnih in nevarnih odpadkov za l. 2006, po dejavnostih, povzročiteljih, vrstah odpadkov in načinih ravnanja. Opaziti je nadaljnji trend povečanega nastajanja odpadkov in neustreznega ravnanja z njimi.
 - Okoljevarstvena karakterizacija žlinder na odpadnih haldah nekdanjega rudnika živega srebra Idrija in sodelovanje pri načrtovanju njihove sanacije. Idrija je eno od okoljsko najbolj obremenjenih mest v Sloveniji zaradi velikih količin površinsko odloženih metalurških odpadkov, ki emitirajo živo srebro v zrak,

- 1 Independent Scientific Contribution in a Monograph
- 1 Published Scientific Conference Contribution
- 1 Published Professional Conference Contribution
- 1 Published Scientific Conference Contribution Abstract
- 6 Treatises, Preliminary Studies, Studies
- 2 Expertises, Arbitration Decisions
- 1 Graduate Thesis
- 1 Master's Thesis
- 2 Journal Editorships

RESULTS IN 2007

- Participation in the integrated EU FP6 project »BIOCOP« named «Energy 3: Co-processing of upgraded bio-liquids in standard refinery units«. The laboratory is engaged in identification of optimal recovery and fractionation strategies and technologies for the production of discrete target compounds from the bio-liquids and development of technically and economically feasible isolation and fractionation technologies for target oxygenate compounds.
- Construction of high pressure view-cell for determination of thermophysical properties of materials and design of related synthesis and separations (in cooperation with Bayer Technology Services, Leverkusen). Cooperation with University of Erlangen, Germany, for microparticle formation of drugs by use of SCF-GAS technique; drug release studies in various environments
- Chapter in the book, describing the developments and applications of solubility. The contribution discusses the importance of physicochemical property data that can be regarded as raw material of chemical process design. The quality of the raw material might strongly affect the quality of the product. This chapter is case oriented, where actual problems from industry are discussed.
- Participation in the optimisation study of a deodorization process, as a final major step

vodo in tla. Izdelan je pregled stanja in podane nekatere rešitve za ravnanje s starimi haldami, kjer se izvajajo večji gradbeni projekti.

- Sodelovanje pri izdelavi tehnoloških podlag za optimiranje novega industrijskega postopka za proizvodnjo čiste fosforne kisline živilske kvalitete ter ravnana s procesnimi ostanki v TKI Hrastnik (v okviru programa Centra odličnosti »Ekološke tehnologije«).
- Uvedba postopkov za vzorčenje in homogenizacijo materialov po standardih SIST EN 14899 in 15002 za potrebe izvajanja sistema vodenja kvalitete po standardu SIST ISO/IEC 17025.

in the refining of an edible oil, by using the appropriate thermodynamic model to describe the multicomponent phase equilibria.

- Upgrade and update of the national information system on waste generation: data collection system for municipal, industrial, construction/demolition and hazardous wastes, generated during the year 2006 in relevant sectors and waste types according to NACE and EWC classification.
- Inventory and environmental impact assessment of waste tailings deposits around the former mercury mine in Idrija; preparation of a related site remediation project (EVT Systems/Kolektor Idrija, Slovenia).



SLIKA 1:
Gradnja naprave za določanje faznih ravnotežij pri visokih tlakih.

FIGURE 1:
Construction of the apparatus for phase equilibria determination at high pressure.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- TKI Hrastnik d.d., Hrastnik;
- JUB d.d., Dol pri Ljubljani;
- Agencija RS za okolje, Ministrstvo za okolje in prostor;
- JP Snaga, Ljubljana in JP Vodovod-kanalizacija, Ljubljana;
- EVT Sistemi d.o.o. in Kolektor d.d., Idrija.

MEDNARODNO SODELOVANJE

- Integrirani EU projekt BIOCOUP v okviru FP6-2004-Energy 3 z naslovom: »Co-processing of upgraded bio-liquids in standard refinery units«: podprojekti SP4 »Production of Discrete Oxygenated Target Compounds« - optimizacija separacijskih strategij ter razvoj

- Participation in the design of industrial solvent extraction plant for production of pure phosphoric acid from wet P.A. (TKI Hrastnik d.d., Chemical Industry, Slovenia); participation in the research of industrial restructuring process (Belinka Chemical factory, Ljubljana, Slovenia); paint waste stabilization (JUB d.d., Dol pri Ljubljani, Slovenia), recovery of municipal waste by treatment and processing (Snaga Ljubljana, Slovenia) etc.
- Participation in the Centre of Excellence (coordinator Joseph 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.



SLIKA 2:
Kombinacija naprav za pripravo testnih vzorcev biomase in mešanih odpadkov: a) rezilni mlin, b) ultracentrifugalni mlin.



FIGURE 2:
Combination of mills for disintegration of laboratory samples of biomass and mixed waste.

separacijskih tehnologij za izolacijo potencialnih frakcij in komponent;

- COST Action C18 " Performance assessment of urban infrastructure services: The case of water supply, wastewater and solid waste", delovna skupina WG3 (trdni odpadki).

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 250 litrov; s pripadajočo infrastrukturo, merilno-regulacijsko opremo, računalniško programsko opremo za načrtovanje procesov ter analizo in obdelavo podatkov; različna oprema za določanje faznih ravnotežij sistemov tekočina - para, tekočina - tekočina in tekočina - trdno za potrebe načrtovanja postopkov destilacije, rektifikacije, ekstrakcije, absorpcije, adsorpcije, sušenja, kristalizacije ipd; programska oprema za modeliranje in vodenje procesov (ASPEN+, GaBi; PROCEDE ...).

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Mentorstva:

1 magistrsko delo, 1 diplomsko delo ter več seminarskih nalog na fakultetah Ljubljanske univerze.

Habilitacije in dejavnosti:

- V. Grilc, izr. prof. za kemijsko in ekološko inženirstvo (Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani). Poučevanje: Gospodarjenje z odpadnimi snovmi (Univerzitetni študij vodarstva in komunalnega inženirstva, Fakulteta za gradbeništvo in geodezijo, Univerza v Ljubljani); Ravnanje z odpadki (FGG – Podiplomski študij komunalne smeri ter Univerza v Ljubljani - Interdisciplinarni podiplomski študij varstva okolja).
- L. Fele Žilnik, znanstvena sodelavka za področje kemijskega inženirstva (Fakulteta za kemijo in kemijsko tehnologijo Univerze v

COLLABORATION WITH COMPANIES AND OTHER PARTNERS

- Pilot-plant experiments, process modelling and optimization (non-catalytic chemical syntheses, component/phase separation, mixing etc.), products upgrading, pollution prevention and waste minimisation studies (for many prominent Slovene chemical factories and other process industries); municipal waste separation and treatment (for some bigger municipal waste management companies).
- 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 modeling of thermodynamic equilibrium of various combination of systems (liquid-vapour, liquid-liquid and liquid-solid), supporting design and calculation of basic unit operations (distillation, extraction, absorption, adsorption, drying, crystallization etc.)

EDUCATION

Supervision of student projects:

1 MSc project

1 BSc projects

Assignments:

- V. Grilc: associate professor in chemical/environmental engineering
- L. Fele Žilnik: research fellow in chemical engineering

Ljubljani). Poučevanje: Vodenje Praktikuma iz kemijskega inženirstva za 4. letnik (Katedra za kemijsko, biokemijsko in ekološko inženirstvo, Fakulteta za kemijo in kemijsko tehnologijo, Univerza v Ljubljani).

(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
prof. dr. Janez Plavec

RAZISKOVALCI / RESEARCHERS

dr. Primož Šket
dr. Christophe Thibaudeau (do 30. 06. 2007)
dr. Igor Zhukov (od 02. 04. 2007)
dr. Simona Golič Grdadolnik (delno / partly)
dr. Gregor Mali (delno / partly)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS

Mirko Cevc
Peter Podbevšek

TEHNIČNO OSEBJE / TECHNICAL STAFF

Aleksandar Gačeša
Damjan Makuc
Gregor Ilc
Marjeta Kebrič (delno / partly)



PODROČJA DEJAVNOSTI

V program delovanja NMR centra za leto 2007 so bile vključene NMR meritve in raziskave za vse uporabnike, ki so se te potrebovali in uporabljali pri svojem raziskovalnem in razvojnem delu v okviru osnovnih in aplikativnih raziskav in projektov za industrijo ali v industriji sami. NMR center upravlja Programski svet v sestavi: prof. dr. Janez Dolinšek (Institut Jožef Stefan, predsednik), dr. Darko Kocjan (Lek, namestnik predsednika), dr. Rok Zupet (Krka), prof. dr. Venčeslav Kaučič (KI), dr. Roman Jerala (KI), prof. dr. Daniel Kikelj (Fakulteta za farmacijo UL), dr. Mitja Kocjančič (Kmetijski inštitut Slovenije), prof. dr. Branko Stanovnik (Fakulteta za kemijo in kemijsko tehnologijo UL), dr. Zoran Šušterič (Sava) in dr. Simona Golič Grdadolnik (MVZT).

Program dela NMR centra za leto 2007 je obravnaval in potrdil Programski svet NMR centra. V letu 2007 je delo NMR centra potekalo v okviru preko 73 programov in projektov. Raziskave v okviru NMR centra so v letu 2007 izvajali raziskovalci naslednjih domačih institucij, ki so soustanoviteljice in sovlagateljice v nakup instrumentov NMR centra: KI, IJS, Fakulteta za farmacijo UL, Fakulteta za kemijo in kemijsko

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 2007 comprised NMR studies and measurements for academic institutions and researchers from industrial partners. Research program of NMR centre includes data acquisition and interpretation for those who apply NMR in their research as part of their research and development projects in academic institutions or in industry itself. Annual research program is discussed and approved by the Scientific council of NMR centre. Current members of the scientific council are: Prof. Dr. Janez Dolinšek (IJS, president), Dr. Darko Kocjan (Lek, vice-president), Dr. Rok Zupet (Krka), Prof. Dr. Venčeslav Kaučič (NIC), Prof. Dr. Roman Jerala (NIC), Prof. Dr. Daniel Kikelj (FP), Dr. Mitja Kocjančič (AIS), Prof. Dr. Branko Stanovnik (FCCT), Dr. Zoran Šušterič (Sava), and Dr. Simona Golič Grdadolnik (Ministry of Higher Education, Science and Technology).

tehnologijo UL in Kmetijski inštitut Slovenije. V zadnjih nekaj letih smo sodelovanje NMR centra na KI razširili na uporabnike z NUKa, Inštituta za hmeljarstvo in pivovarstvo Slovenije, Naravoslovno-tehnične, Biotehniške in Medicinske fakultete Univerze v Ljubljani ter Univerze v Novi Gorici. Instrumenti so na razpolago vsem ustanovam in podjetjem, ki jih potrebujejo pri svojem delu. Podjetja Lek, Krka in Helios jih kot sovlagatelji pri nakupu osnovne opreme NMR centra uporabljajo pri rutinski analitiki in v okviru svojega raziskovalno-razvojnega dela. V letu 2007 so instrumente v okviru NMR centra na KI uporabljali tudi raziskovalci iz podjetij Fenolit in TKK.

Raziskave v NMR centru so obsegale:

- študij struktur oligomernih fragmentov nukleinskih kislin ter konformacijskih sprememb gradnikov DNK ob interakciji s kovinskimi ioni;
- študij struktur in dinamike proteinov, zvižanja proteinov in molekularnih interakcij peptidov z lipopolisaharidi;
- študij interakcij med ligandi in receptorjem;
- študij struktur in dinamike antibiotikov v povezavi z njihovim biološkim učinkom;
- raziskave struktur in dinamike organskih molekul, detekcija in karakterizacija reaktivnih intermediatov pri reakcijah organskih in organokovinskih spojin;
- študij naravnih produktov;
- študij sprememb v eritrocitih med bolezenskimi stanji;
- študij struktur 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 struktur in čistosti polimernih materialov, vsebnosti stranskih produktov polimerizacije, mehanizmov polimerizacije,

In 2007 the cooperation between various research groups and NMR centre at NIC involved over 73 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 Jožef Stefan, Faculty of Pharmacy of University of Ljubljana, Faculty of Chemistry and Chemical Technology of University of Ljubljana and Agricultural Institute of Slovenia. In the last few years cooperation of NMR centre at NIC has been extended to National University Library, The Slovenian Institute for Hops Research and Brewing, Faculty of Natural Sciences and Engineering of University of Ljubljana, Faculty of Biotechnology of University of Ljubljana, Faculty of medicine of University of Ljubljana and University of Nova Gorica. NMR spectrometers are available to all institutions and companies which apply NMR spectroscopy at their R&D. Companies Lek, Krka and Helios use NMR spectrometers as analytical tool as well as in their research and development projects. In 2007 NMR centre offered services and help to companies Fenolit and TKK.

Research activities of NMR centre included studies of:

- structure of oligomeric nucleic acids fragments and conformational changes in DNA upon interaction with metal ions,
- protein structure and dynamics, protein folding and molecular interactions of peptides with lipopolysaharides,
- ligand-receptor interactions,
- structure and dynamics of antibiotics in relation with their biological role,
- structure and dynamics of organic molecules, detection and characterization of reactive intermediates in reactions of organic and organometallic compounds,
- natural products,
- changes in erythrocytes during disease,

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, magistririjev in doktoratov.

BIBLIOGRAFIJA

- 6 izvirnih znanstvenih člankov
- 1 strokovni članek
- 1 objavljeni znanstveni prispevek na konferenci
- 9 objavljenih povzetkov znanstvenih prispevkov na konferencah
- 1 predavanje na tuji univerzi
- 1 prispevek na konferenci brez natisa
- 2 vabljeni predavanji na konferencah brez natisa

GLAVNI DOSEŽKI V LETU 2007

Raziskovalni dosežki, ki so nastali v sodelovanju NMR centra z raziskovalnimi laboratoriji in skupinami širom po Sloveniji so bili objavljeni v mnogih publikacijah v revijah z mednarodnim recenzentskim sistemom (seznam je dostopen na domači strani NMR centra na naslovu www.nmr.ki.si). Precejšnje število teh dosežkov je bilo objavljenih v revijah, ki segajo v 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 preko uspešnega poslovnega rezultata posameznega podjetja.

V letu 2007 smo zaključili dve študiji struktur z gvanini bogatih oligonukleotidov. Molekulo $d[G_4(T_4G_4)_3]$ smo zvali v unimolekularno G-kvadrupleksno strukturo v prisotnosti ^{15}N -označenih amonijevih ionov. S pomočjo NMR spektroskopije smo dokazali, da je topologija enaka strukturi predhodno določeni v prisot-

- structure and conformational equilibria of metabolites in solution and in solid state,
- determination of byproducts in pharmaceuticals and their metabolites,
- structural characterization of phosphate based porous materials and structural changes in the process of hydrothermal synthesis of zeolites,
- structure and purity of polymers, byproducts of polymerization, mechanisms of polymerization and properties of polymers with designed macromolecular structure,
- determination of authenticity, quality and origin of Slovenian wines.

NMR centre has important role in education and training. NMR centre offers collection, and interpretation of NMR spectra on specific structural problems that are part of bachelor, masters and doctoral thesis.

BIBLIOGRAPHY

- 6 Original Scientific Articles
- 1 Professional Article
- 1 Published Scientific Conference Contribution
- 9 Published Scientific Conference Contribution Abstracts
- 1 Invited Lecture at Foreign University
- 1 Unpublished Conference Contribution
- 2 Unpublished Invited Conference Lectures

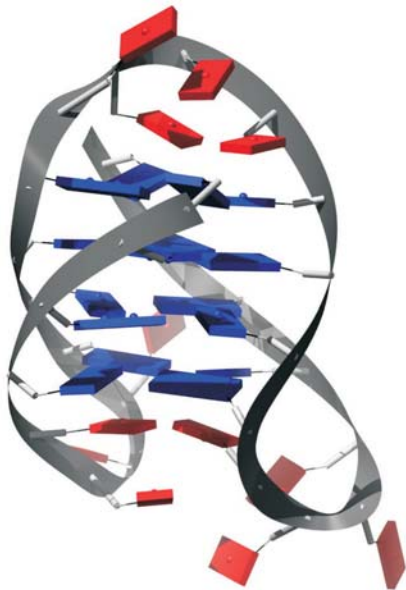
IMPORTANT ACHIEVEMENTS IN 2007

Scientific achievements, which are the result of cooperation of NMR center with laboratories and groups around Slovenia were published in many publications in journals with international peer review evaluation procedure (complete list is available on NMR center's home-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

nosti Na^+ ionov. $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$ kvadrupleks je sestavljen iz štirih G-kvartetov, ki definirajo tri kationska vezavna mesta (O_1 , I in O_2). Obravnavali smo izmenjavo amonijevih ionov znotraj $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$ kvadrupleksa in z okoliško raztopino. Izmenjavi smo sledili z uporabo 2D ^1H - ^{15}N korelacijskih eksperimentov. Ugotovili smo, da se $^{15}\text{NH}_4^+$ ioni znotraj G-kvadrupleksa ne gibljejo le v eni smeri ali "v gosjem redu", kot je značilno za ionske kanale. Amonijevi ioni se izmenjujejo med tremi vezavnimi mesti, ki se nahajajo med pari sosednjih G-kvartetov. Ker je amonijev ion prevelik, da bi lahko prosto prehajal skozi osrednjo odprtino G-kvartetov se morajo le ti ob prehodu iona delno razpreti. Posledično je hitrost izmenjave skozi posamezen G-kvartet odvisna od njegove rigidnosti. Izmenjava amonijevih ionov z okolico je hitrejša kot izmenjava znotraj G-kvadrupleksa in je odvisna od strukture povezovalnih zank. Sterične

institutes or faculties. Results of cooperation between NMR center and Slovenian industry are publicly known only through positive financial results of individual company.

We have completed two studies of structures of guanine-rich oligonucleotides in 2007. $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$ has been folded into the unimolecular G-quadruplex in the presence of ^{15}N -labelled ammonium ions. The use of NMR data has enabled us to demonstrate that its folding topology is equivalent to the 3D structure established earlier in the presence of Na^+ ions. $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$ quadruplex exhibits four G-quartets which define three cation binding sites (O_1 , I in O_2). We have studied the exchange of ammonium ions within the unimolecular G-quadruplex $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$ and with bulk solution. Exchange was followed with the use of 2D NMR experiments and ^{15}N -labeled ammonium ions. We established that, unlike in ion channels,



SLIKA 1:

Shematski prikaz G-kvadrupleksa $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$. Gvaninski preostanki (prikazani v modri barvi) so sestavni del štirih G-kvartetov, med katerimi se nahajajo tri vezavna mesta za amonijeve ione. Timidini (prikazani v rdeči barvi) tvorijo na eni strani strukture diagonalno zanko, na nasprotni strani pa dve robni zanki.

FIGURE 1:

Schematic representation of $d[\text{G}_4(\text{T}_4\text{G}_4)_3]$ quadruplex. Guanine residues (colored blue) are the building blocks of the four G-quartets which define the three ammonium ion binding sites between them. Thymidines (colored red) on one side of the G-quadruplex form a diagonal loop and two edge-wise loops on the opposite side of G-quadruplex core.

omejitve dveh robnih T_4 zank na eni strani strukture nasproti diagonalni T_4 zanki na drugi strani strukture so rezultirale v petkratni razliki v hitrosti izmenjave amonijevih ionov. Izsledke te študije smo objavili v reviji Nucl. Acids Res. Posvetili smo se tudi študiji dinamike $^{15}\text{NH}_4^+$ ionov znotraj $d[(G_3T_4G_4)_2]$ kvadrupleksa. Njegova struktura je dimerna in vsebuje tri G-kvartete in dve T_4 zanki. Znotraj tega G-kvadrupleksa smo identificirali dve kationski vezavni mesti, ki smo ju poimenovali U in L. Presenetljivo je, da nismo opazili gibanja kationov vzdolž centralnega ionskega kanala tega G-kvadrupleksa. Pomemben aspekt študij interakcij kovinskih ionov z nukleinskimi kislinami je razumevanje njihovih dinamičnih lastnosti. Do sedaj objavljeni rezultati kažejo, da se kationi izmenjujejo med vezavnimi mesti znotraj G-kvadrupleksa, kar bi lahko vodilo do njihove uporabe kot ionskih kanalov. Naša študija pa je pokazala, da je v preiskovani molekuli izmenjava kationov znotraj G-kvadrupleksa onemogočena. Opazili smo le izmenjavo amonijevih ionov z ioni iz raztopine. Opažanja smo razložili s strukturnimi značilnostmi študirane molekule. Izmenjava amonijevih ionov preko zunanega G-kvarteta, ki ga premošča timidinska zanka, ki poteka po njegovem robu je 12x hitrejša od izmenjave preko G-kvarteta, ki ga premošča diagonalna T_4 zanka. Razumevanje vpliva različnih orientacij zank na hitrost izmenjave $^{15}\text{NH}_4^+$ ionov, je pomembno pri uvedbi bolj splošnih pravil o tem, katero od zunanjih vezavnih mest bo imelo hitrejšo izmenjavo kationov. Takšno znanje je ključno pri načrtovanju sintetskih ionskih kanalov na osnovi G-kvadrupleksnih struktur. Rezultate te študije smo objavili v J. Am. Chem. Soc.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

NMR center je infrastrukturni center, ki nudi podporo najširšemu krogu akademskih in ostalih uporabnikov. Zelo intenzivni so stiki z naslednjimi industrijskimi partnerji, ki so

there is no unidirectional ion movement in a single file within the G-quadruplex. Ammonium ions were shown to move between three binding sites which were localized between pairs of two adjacent G-quartets. As ammonium ions are too big to move freely through the central cavity of G-quartets, the G-quartets have to slightly open upon passage. As a result the exchange rate through an individual G-quartet is in direct relation with its stiffness. Exchange with bulk solution is faster than exchange within the G-quadruplex and is related to the structure of the connecting loops. Steric hindrance posed by the two lateral T_4 loops on one side of the structure with respect to the diagonal T_4 loop on the other side of the G-quadruplex core results in five-fold difference in the exchange rate of ammonium ions. The results of these study were published in Nucl. Acids Res.

The focus of our other published study was the dynamics of movement of $^{15}\text{NH}_4^+$ ions within $d[(G_3T_4G_4)_2]$ quadruplex. This dimeric G-quadruplex structure consist of three G-quartets and two T_4 loops. We were able to establish two cation binding sites, named U and L, within the interior of $d[(G_3T_4G_4)_2]$. Studies concerning interactions between metal ions with nucleic acids are essential for understanding of their dynamic properties. All results available in the literature up to now showed that cations within G-quadruplex structures are not bound statically, which has stimulated explorations of G-quadruplexes as ion channels. Surprisingly there is no cation movement along the central ion cavity of this G-quadruplex. Our unique observations were interpreted in terms of structural features of $d[(G_3T_4G_4)_2]$ quadruplex. On the other hand, we have observed exchange of ammonium ions with ions in bulk solution. $^{15}\text{NH}_4^+$ ion movement through the outer G-quartet that is spanned by the edge-wise T_4 loop is 12 times faster than through the outer G-quartet which is spanned by the diagonal T_4 loop. An understanding of the influence of different loop orientations on the rate of $^{15}\text{NH}_4^+$ ion movement is important to establish more

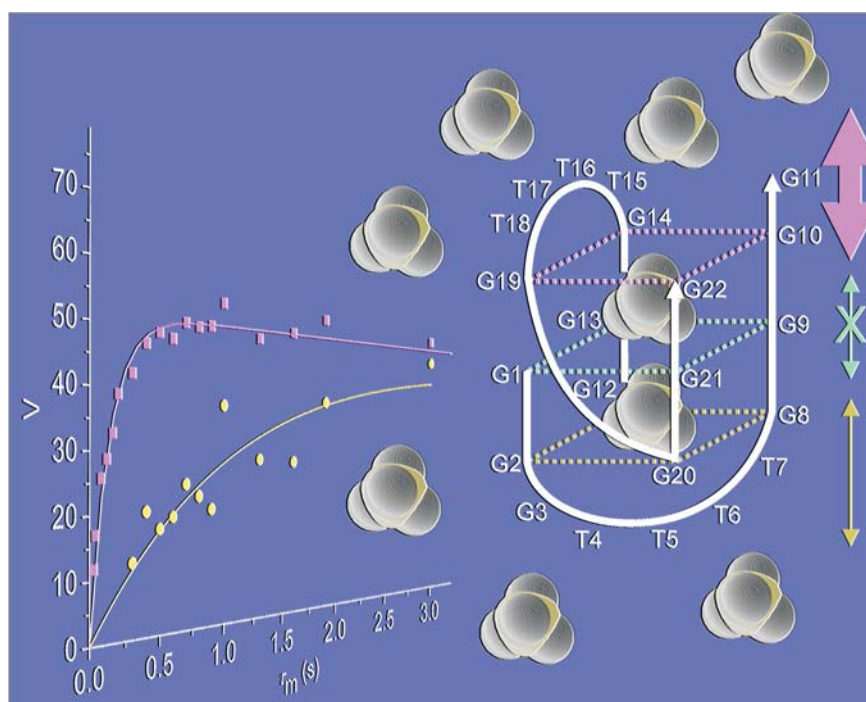
sovlagatelj v opremo NMR centra:

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

Ostali industrijski uporabniki uslug NMR centra v letu 2007 so bili:

- Fenolit d.d., Borovnica;

general rules with the ultimate aim to predict which of the outer cation binding sites will exhibit faster ion movement. Such knowledge is expected to guide future efforts to build synthetic ion channels based on G-quadruplex structures. The results of these study were published in J. Am. Chem. Soc.



SLIKA 2:

Lokalizacija dveh amonijevih ionov znotraj bimolekularnega $d[(G_3T_4G_4)_2]$ G-kvadrupleksa sestavljenega iz treh G-kvartetov. Dva zunanja G-kvarteta sta povezana z eno diagonalno in eno zanko, ki poteka po robu. Puščice ob robu prikazujejo smer in učinkovitost oz. hitrost izmenjave $^{15}\text{NH}_4^+$ ionov. Posebej zanimivo je, da izmenjava med vezavnima mestoma znotraj G-kvadrupleksa ne poteka. Graf na levi prikazuje odvisnost relativnih volumnov korelacijskih signalov v seriji 2D ^1H - ^{15}N heteronuklearnih NMR spektrov od t.i. mešalnega časa NMR eksperimenta. Dva seta podatkov in dve krivulji v grafu ustrežata premikanju $^{15}\text{NH}_4^+$ ionov iz dveh vezavnih mest v okoliško raztopino.

FIGURE 2:

Localization of two ammonium ions within bimolecular $d[(G_3T_4G_4)_2]$ G-quadruplex structure composed of three G-quartets. Two outer G-quartets are spanned with one diagonal and one edge-wise loop. Arrows on the right-hand side of the structure indicate directions and effectiveness (rate) of $^{15}\text{NH}_4^+$ ion exchange. It is noteworthy that there is no exchange between the two cation binding sites within the G-quadruplex. The graph of the left-hand side shows relative volume intensities of cross-peaks in a series of 2D ^1H - ^{15}N heteronuclear NMR spectra as a function of mixing time of the NMR experiment. Two sets of data points and two best fit curves correspond to $^{15}\text{NH}_4^+$ ion movement from the two binding sites into bulk solution.

- TKK Serpenica d.d., Srpenica.

MEDNARODNO SODELOVANJE

Mednarodno sodelovanje NMR centra je obsežno (seznam mednarodnih projektov je dostopen na www.nmr.ki.si).

POMEMBNI INSTRUMENTI IN OPREMA

V okviru NMR centra na lokaciji KI so nameščeni sledeči NMR spektrometri visoke ločljivosti:

- Varian NMR systems 800;
- Varian NMR systems 600;
- Varian Unity Inova 300;
- Varian Unity Inova 300.

Zadnja velika posodobitev opreme je bila izvedena s pomočjo sredstev Evropskega sklada za regionalni razvoj.

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

Pomemben vidik delovanja NMR centra je njegova izobraževalna vloga. NMR center nudi pomoč pri snemanju in interpretaciji NMR spektrov pri konkretnih strukturnih problemih v okviru diplomskih del, magisterijev in doktoratov.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

NMR centre plays a role of infrastructural facility and as such offers its support and expertise in the field of NMR spectroscopy to all interested academic research institutions as well as to commercial companies. The following industrial partners have participated in the purchase of the equipment and are regular users of NMR facility:

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

The other industrial users of our services and expertise in 2007 were:

- Fenolit d.d., Borovnica, Slovenia;
- TKK Serpenica d.d., Srpenica, Slovenia.

INTERNATIONAL COLLABORATION

NMR centre is involved in extensive international collaboration. List of international projects is available at www.nmr.ki.si.

MAJOR EQUIPMENT

Major equipment of NMR centre includes the following high-resolution NMR spectrometers:

- Varian NMR systems 800;
- Varian NMR systems 600;
- Varian Unity Inova 300;
- Varian Unity Inova 300.

We are proud to note that the latest upgrade of research equipment was made possible with the financial support of European Regional Development Funds.

EDUCATION AND IMPORTANT VISITS

Important aspect of NMR centre's activity is its role in education. NMR centre offers help at collection and interpretation of NMR spectra on specific structural problems that are part of bachelor, masters and doctoral thesis.

L16

Center za validacijske tehnologije in
analitiko (CVTA)

Centre for Validation Technologies and
Analytics (CVTA)



VODJA / HEAD

doc. dr. Janko Žmitek (Sektor skupnih služb /
General Sector)

RAZISKOVALCI / RESEARCHERS

Sodelavci iz L06 – odgovorni nosilci nalog / as-
sociates from L06:

dr. Mirko Prošek (vodja področja / head of pro-
gram)

dr. Alenka Golc Wondra (vodja področja / head
of program)

Mitja Križman

dr. Andrej Šmidovnik

TEHNIČNO OSEBJE / TECHNICAL STAFF

Ana Andrić

Katarina Jankovič

Adolf Krašna

Darija Lorber

Katja Rožmanc Babnik

Barbara Lečnik Spaić

Renata Ciglarič (do / untill 15. 7. 2007)

Simona Lojvec (od / since 13. 8. 2007)



PODROČJA DEJAVNOSTI

CVTA načrtuje in izvaja razvojno-analitske storitve na področju zdravil in prehrane; njegova dejavnost obsega:

- razvoj HPLC, GC, TLC in drugih analiznih postopkov ter postopkov za določanje hitrosti raztapljanja;
- načrtovanje in izvedbo validacij analiznih postopkov;
- izvajanje analiz in analiznih študij za potrebe kontrole kakovosti izdelkov ter validacij proizvodnih tehnologij in tehnologij čiščenja proizvodne opreme;
- izvajanje analiz za študij biorazpoložljivosti oz. bioekvivalentnosti zdravil;
- validacije analiznih metod in tehnologij z navedenimi tehnikami;
- izdelavo ekspertnih mnenj in svetovanja na področju dejavnosti.

Aktivnosti potekajo v skladu s standardi dobre laboratorijske oz. dobre proizvodne prakse.

GLAVNI DOSEŽKI V LETU 2007

CVTA sledi naraščajočim potrebam slovenske in tuje farmacevtske industrije po analitski podpori razvojnim in proizvodnim projektom ob

RESEARCH 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 2007

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. All the activities were performed in tight collaboration with L06, which offered professional support of its experts to CVTA.

Crucial achievements in the year 2007 are:

zaostrovanju kakovostnih zahtev za izvajanje takšnih del. Delo v CVTA poteka ob strokovni podpori Laboratorija za prehrabno kemijo (L06).

V l. 2007 smo za slovensko farmacevtsko industrijo izvedli:

- razvoj 14 analitskih postopkov;
- validacijo 35 HPLC, GC in TLC analitskih postopkov;
- analize za validacijo in kontrolo 9 proizvodnih tehnologij;
- analize za validacije in kontrolo ca. 20 tehnologij čiščenja proizvodne opreme;

- Development of 14 analytical methods;
- Validation of 35 HPLC, GC in TLC analytical methods;
- Analyses for 9 process validations;
- Analyses for ca 20 cleaning validations;
- Analyses for several stability studies;
- Analyses of residual solvents (OVI) in approximately 800 samples of pharmaceutical finished dosage forms;
- Analyses of different parameters of ca 200 other samples.

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



SLIKA:

Nekaj izmed izdelkov, obogatenih z vodotopnim koencimom Q10, izdelanih po licenci Kemijskega inštituta

FIGURE:

Food products enriched with water soluble Coenzyme Q10, prepared according to the licence of the National Institute of Chemistry

- analize v okviru stabilitetnih študij za več preparatov;
- analize rezidualnih topil v ca. 800 vzorcih različnih preparatov;
- analize različnih parametrov za ca. 200 drugih vzorcev.

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. 2007 ustvaril z delom za farmacevtsko industrijo, zlasti z družbama Lek in Krka.

POMEMBNI INSTRUMENTI IN OPREMA

Štirje HPLC sistemi, trije GC sistemi 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, the member of Sandoz company, and Krka.

MAJOR EQUIPMENT

Four HPLC systems, three 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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L02

Laboratorij za spektroskopijo materialov

Laboratory for Spectroscopy of Materials

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L03

Laboratorij za kemometrijo

Laboratory of Chemometrics

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

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16. NOVIČ, Marjana. Kohonen and counter-propagation neural networks applied for mapping and interpretation of IR spectra. V: LIVINGSTONE, David (ur.). Artificial neural networks : methods and applications. Humana Press, 2007, str. [1-15]. [COBISS.SI-ID 3836442]

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L04

Laboratorij za analizno kemijo

Analytical Chemistry Laboratory

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

1. BEESTON, M.P., GLASS, Hylke J., ELTEREN, Johannes Teun van, ŠLEJKOVEC, Zdenka. Assessment of elemental mobility in soil using a fluidised bed approach with on-line ICP-MS analysis. *Anal. Chim. Acta*, 2007, vol. 599, no. 2, str. 264-270. [COBISS.SI-ID 20986919]
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Mentorstva / Mentorships

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L05

Laboratorij za kemijo, biologijo in tehnologijo vod

Laboratory for Chemistry, Biology and Technology of Water

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

1. BERDEN ZRIMEC, Maja, DRINOVEC, Luka, ZRIMEC, Alexis, TIŠLER, Tatjana. Delayed fluorescence in algal growth inhibition tests. *Cent. Eur. J. Biol.*, 2007, vol. 2, no. 2, str. 169-181. [COBISS.SI-ID 3702042]
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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)

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L07

Laboratorij za polimerno kemijo in tehnologijo

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L08

Laboratorij za organsko sintezo in kemijo zdravil

Laboratory for Organic and Medicinal Chemistry

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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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L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry

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L13

Laboratorij za katalizo in reakcijsko inženirstvo

Laboratory for Catalysis and Chemical Reaction Engineering

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

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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

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