Poročilo o delu 2004

Annual report 2004

POROČILO O DELU 2004 / ANNUAL REPORT 2004

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Ljubljana, 2005

Kazalo

Index

Beseda direktorja

Word of the Director

Na Kemijskem inštitutu smo v lanskem letu uspešno uresničevali naše poslanstvo pridobivanja novih znanj z vrhunskim raziskovalnim delom in posredovanja pridobljenih znanj v družbo.

Na Kemijskem inštitutu želimo ustvarjati stimulativno raziskovalno okolje, v katerem si raziskovalci postavljajo visoke raziskovalne cilje na aktualnih interdisciplinarnih področjih. Zgolj povprečnost na javni raziskovalni instituciji ni sprejemljiva! Za doseganje visokega nivoja raziskav so ključni motivirani sodelavci in kvalitetni pogoji dela. Primerjalna študija Skupnega raziskovalnega centra evropskih raziskovalnih inštitutov je pred nekaj leti pokazala, da je Kemijski inštitut povsem primerljiv z najuglednejšimi inštituti v Evropi po večini izbranih parametrov. Razloge za to gre vsekakor iskati v sposobnih raziskovalcih na inštitutu ter učinkovitem vodenju, saj so finančna sredstva na raziskovalca na Kemijskem inštitutu celo 3 do 4 krat manjša kot na inštitutih

Last year the National Institute of Chemistry successfully fulfilled its mission of acquiring new knowledge through high - level research work and of sharing this knowledge with the wider society.

At the National Institute of Chemistry we wish to create a stimulating research environment in which researchers can set high goals for research in contemporary interdisciplinary areas. Being average is simply not acceptable at a public research institution! The keys to reaching a high level of research work are motivated people and quality working conditions. A comparative study carried out a few years ago by the Joint Research Centre of European Commission showed that the National Institute of Chemistry is comparable with the most prestigious institutes in Europe, according to the majority of chosen parameters. There are several reasons for this, among which are capable researchers at the Institute and effective leadership, since the financial resources per researcher at our Institute

v bolj razvitih evropskih državah. Tako je pokazala že omenjena primerjalna študija, pa tudi statistični podatki Evropske komisije, zbrani v knjižici Key Figures 2003 - 2004. Ob tolikšni razliki prihodkov je seveda težko ustvariti primerljive pogoje dela ter pritegniti najsposobnejše in ambiciozne raziskovalce, ki naj bi prispevali tudi k hitrejšemu gospodarskemu razvoju Slovenije.

Ustvarjanje pogojev za hitrejši razvoj inštituta je v opisanih ekonomskih okoliščinah toliko večji izziv. Potrebno je stalno dokazovanje kvalitete znanstvenega dela, tekmovanje za industrijske, nacionalne in mednarodne projekte in predvsem graditev partnerskega odnosa z organizacijami, s katerimi sodelujemo.

Kemijski inštitut je svoje razvojne ambicije jasno opredelil v svojem poslanstvu. Za doseganje nadpovprečnih rezultatov so nujne tudi strateške usmeritve inštituta na daljši rok, saj so človeški viri in finančna sredstva omejena, vidnejši znanstveni rezultati pa danes niso možni brez usklajenega večletnega sodelovanja vsaj nekaj raziskovalcev. V letu 2005 bomo zato nadaljevali z opredeljevanjem strateških usmeritev inštituta, kar v obstoječem sistemu ni tako enostavno. Posebej zahtevno je oblikovanje usmeritev inštituta ob pomanjkljivo definiranih nacionalnih prioritetah na področju raziskav in v sistemu javnega financiranja raziskav, kjer inštitut kot celota ne prejema nobenih raziskovalnih sredstev. Javna sredstva za raziskave lahko inštitut pridobi le preko razpisov za manjše projekte ali programe posameznih raziskovalnih skupin.

Pretekle usmeritve in dobro delo sodelavcev so pripomogli k hitremu razvoju in večji prepoznavnosti inštituta. Od leta 1999 smo povečali finančne prihodke v tolarjih za 93 % (57 % v evrih). Dodatna finančna sredstva, kvalitetni znanstveni rezultati in dobro sodelovanje s partnerji so omogočili, da smo bili skupaj uspešni tudi pri nabavi večje in dražje razis-

are 3-4 times less than at institutes in more developed European countries. This is further shown by the previously cited comparative study, as well as by statistical data from the European Commission taken from the booklet Key Figures 2003 - 2004. With such differences in incomes it is difficult to create comparable working conditions and to attract the most able and ambitious researchers in order to contribute to faster economic development in Slovenia.

Creating the conditions for faster development of the Institute is an even greater challenge given the economic environment described above. It is necessary to constantly demonstrate the quality of scientific work, compete for industrial, national, and international projects, and, above all, build strong partnerships with the organizations with whom we cooperate.

The National Institute of Chemistry has clearly defined its development ambitions in its mission statement. In order to reach above average results, long term strategic goals are absolutely necessary, since human and financial resources are limited and tangible scientific results are not possible today without concerted multi - year cooperation by a group of researchers. Thus, we will continue to define the strategic goals of the Institute in 2005, which is a demanding task within the existing set-up. It is particularly difficult to formulate goals for the Institute without defined national priorities for research and within the system of public financing of research, since the Institute as a whole does not receive any research funding. Public research funding can only be obtained by the Institute through proposals for smaller projects or through programs by individual research groups.

Good work by the various collaborators and strong goals in the past have led to faster development and greater recognition of the Institute. Since 1999 we have increased out financial income in tolars by 93 % (57 % in euros).

kovalne opreme. V letu 2004 smo glede na preteklo leto povečali sredstva za nabavo raziskovalne opreme za 75 % in ob podpori industrijskih partnerjev podpisali pogodbo za posodobitev Nacionalnega centra za NMR spektroskopijo visoke ločljivosti. Spomladi 2005 bomo končali z gradnjo infrastrukturnega centra, ki bo namenjen večji raziskovalni opremi. Že jeseni 2005 v novem objektu načrtujemo zagon novega 800 MHz NMR spektrometra in visoko ločljivega praškovnega rentgenskega difraktometra.

Zadovoljni smo z rezultati raziskovalnega dela in sodelovanjem z našimi partnerji v letu 2004. Doseženi rezultati so dobra osnova za še višje postavljene cilje v letu 2005 in v prihodnje. Prepričan sem, da jih bomo s skupnimi napori uresničili v naše skupno zadovoljstvo.

Additional financial resources, high quality scientific results, and good cooperation with our partners have allowed us to successfully acquire larger and more expensive pieces of research equipment. In 2004 we increased the resources dedicated to acquiring new equipment by 75 % compared with the previous year and signed a contract to modernize the National Centre for High Resolution NMR Spectroscopy with the help of our industrial partners. By spring 2005 we will have finished building an infrastructure centre designed for larger pieces of research equipment. In the fall of 2005 we plan to start up a new 800 MHz NMR spectrometer and a high resolution powder x-ray diffractometer in the new building.

We are very pleased with the results of our research work and the cooperation with our partners in 2004. The attained results are a good basis for the even higher goals set for 2005 and for those to be set in the future. I am certain that with a collective effort we will realize these goals to our satisfaction.

dr. Peter Venturini

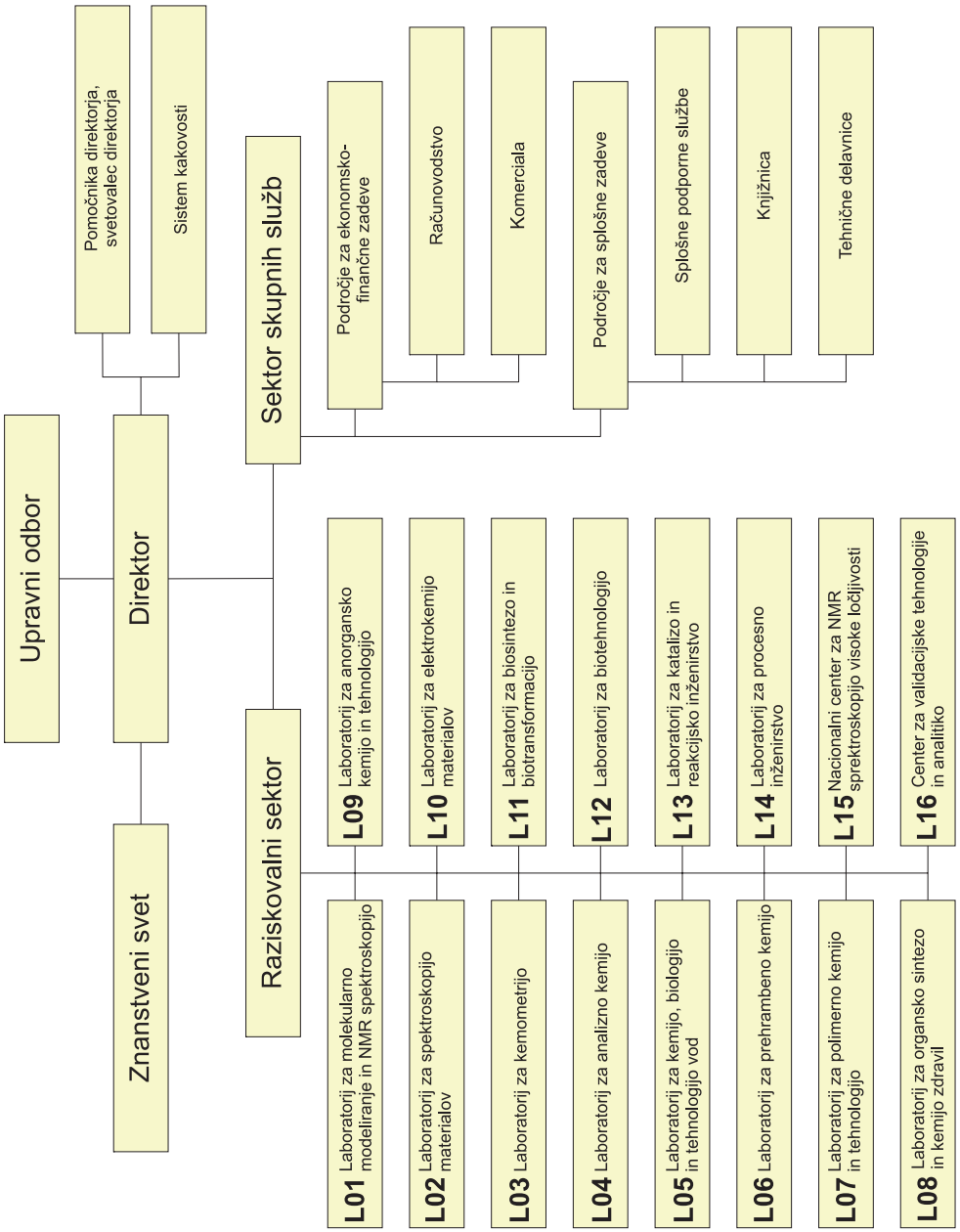
Poslanstvo Kemijskega inštituta

The Mission of the National Institute of Chemistry

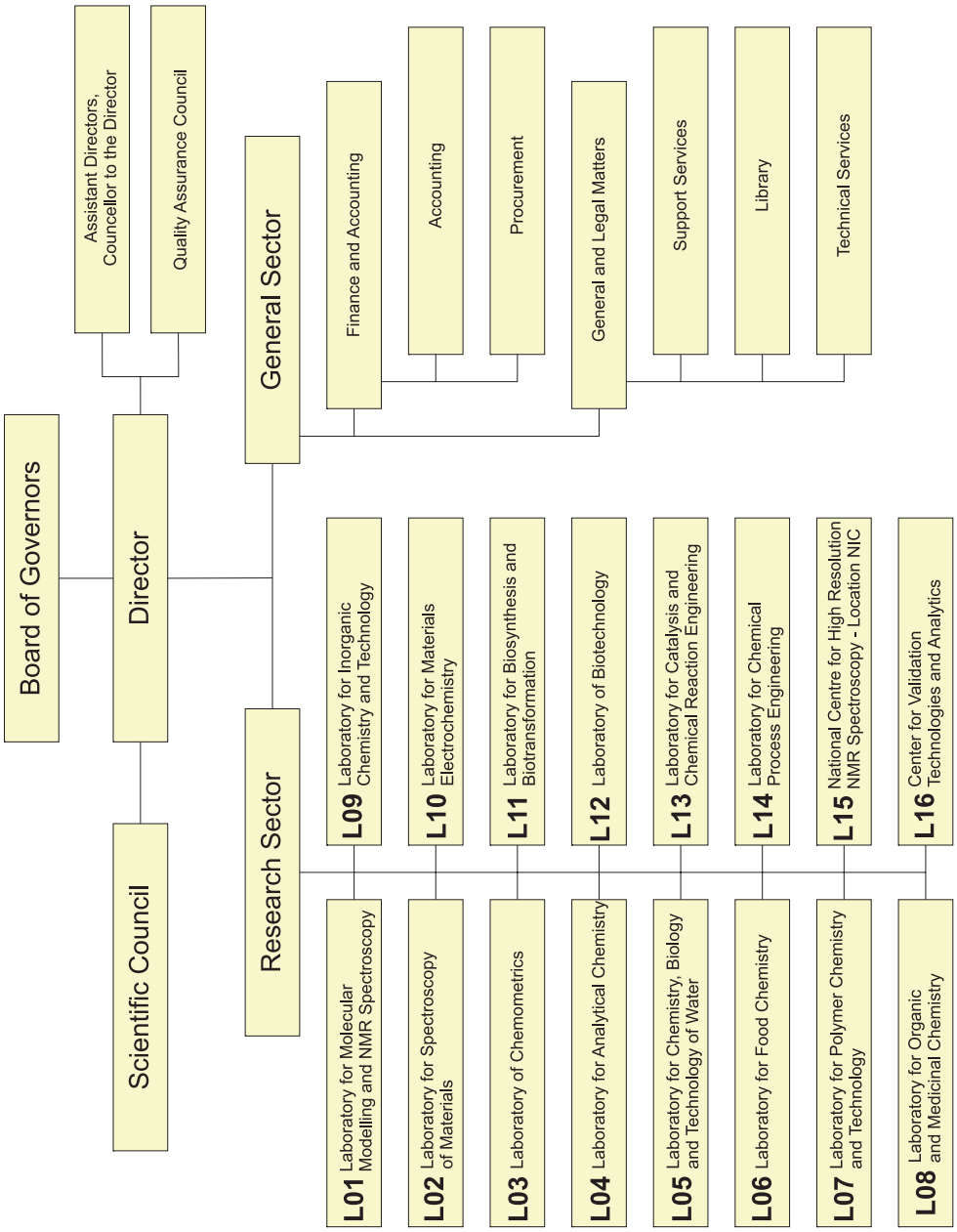
- Kemijski inštitut je v Sloveniji vodilna in v svetu prepoznavna raziskovalna organizacija na področju kemije in sorodnih disciplin.
- Z raziskovalnim delom in moderno infrastrukturo zagotavlja vrhunske znanstveno - raziskovalne dosežke, vzgojo kadrov in prenos novih znanj v gospodarstvo.
- Kemijski 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 achievments, 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**
  Dr. Peter VENTURINI

- **Pomočnika direktorja / Assistant directors**
  Alenka PUKL
  Mag. Janez TOPLIŠEK

- **Svetovalec direktorja / Councellor to the director**
  Doc. dr. Janko ŽMITEK

ČLANI UPRAVNEGA ODBORA / BOARD OF GOVERNORS

- Dr. Stojan Sorčan, predsednik / president
- Dr. Ilija Dimitrievski (od / since 18. 8. 2004)
- Dr. Ljudmila Fele Žilnik (do / until 19. 7. 2004)
- Akad. prof. dr. Dušan Hadži
- Prof. dr. Miha Japelj (do / until 17. 8. 2004)
- Doc. dr. Roman Jerala (od / since 20. 7. 2004)
- Dr. Andrej Kržan (od / since 20. 7. 2004)
- Prof. dr. Ivan Leban
- Dr. Brina Ornik
- Doc. dr. Janez Plavec (do / until 19. 7. 2004)
- Dr. Matjaž Polak
- Dr. Aleš Rotar (od / since 18. 8. 2004)
- Akad. prof. dr. Branko Stanovnik (do / until 17. 8. 2004)

ČLANI ZNANSTVENEGA SVETA / SCIENTIFIC COUNCIL

- Akad. prof. dr. Janez Levec, predsednik / president
- Dr. Janez Jamnik
- Prof. dr. Venčeslav Kaučič
- Prof. dr. Radovan Komel
- Doc. dr. Janez Mavri
- Dr. Marjana Novič
- Doc. dr. Janez Plavec
- Dr. Mirko Prošek
- Prof. dr. Milenko Roš

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 MODIC†, 19. 12. 1986
- Prof. dr. Tihomir NOVAKOV, 19. 12. 1986
- Prof. dr. Robert LAFFERTY, 15. 6. 1994
- Prof. dr. Walter STEINER, 15. 6. 1994
- Prof. dr. D. Luc MASSART, 8. 3. 1995
- Prof. dr. John R. HELLIWELL, 21. 10. 1996
- Prof. dr. Joachim MAIER, 17. 4. 1996
- Prof. dr. Dušan HADŽI, 9. 10. 2001

Finance

PRIHODKI (1000 SIT)

	2003	2004	Struktura 2004 (%)	Indeks 2004/2003
Raziskovalni programi	736.252	835.312	34,7	113,5
Infrastrukturni programi	57.916	99.539	4,1	171,9
Raziskovalni projekti	174.638	272.827	11,3	156,2
Ustanoviteljske obveznosti	351.978	392.287	16,3	111,5
Mladi raziskovalci	216.675	198.729	8,3	91,7
Domači trg	396.461	399.857	16,6	100,9
Tuji trg	192.079	124.843	5,2	65,0
Drugi prihodki	102.542	81.129	3,4	79,1
SKUPAJ PRIHODKI	2.228.541	2.404.523	100,0	107,9

ODHODKI (1000 SIT)

	2003	2004	Struktura 2004 (%)	Indeks 2004/2003
Stroški materiala	-208.475	-247.922	10,7	118,9
Stroški storitev	-289.664	-317.147	13,7	109,5
Amortizacija	-219.473	-230.183	9,9	104,9
Stroški dela	-1.397.790	-1.459.714	63,0	104,4
Drugi odhodki	-36.596	-61.953	2,7	169,3
SKUPAJ ODHODKI	-2.151.998	-2.316.919	100,0	107,7

REZULTAT POSLOVANJA	76.543	87.604	-	114,5

Finances

REVENUES (1000 SIT)

	2003	2004	Structure 2004 (%)	Index 2004/2003
Research programmes	736.252	835.312	34,7	113,5
Infrastructure programmes	57.916	99.539	4,1	171,9
Research projects	174.638	272.827	11,3	156,2
Overhead financing	351.978	392.287	16,3	111,5
Young researchers	216.675	198.729	8,3	91,7
Domestic market	396.461	399.857	16,6	100,9
Foreign market	192.079	124.843	5,2	65,0
Other incomes	102.542	81.129	3,4	79,1
TOTAL	2.228.541	2.404.523	100,0	107,9

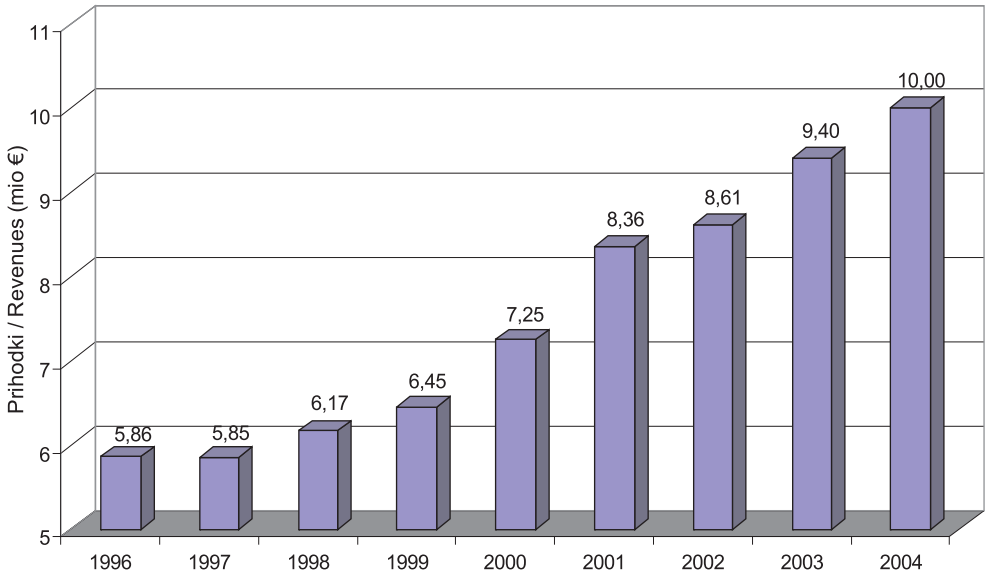
OUTFLOW (1000 SIT)

	2003	2004	Structure 2004 (%)	Index 2004/2003
Costs of material	-208.475	-247.922	10,7	118,9
Costs of services	-289.664	-317.147	13,7	109,5
Depreciation	-219.473	-230.183	9,9	104,9
Labour costs	-1.397.790	-1.459.714	63,0	104,4
Other outcomes	-36.596	-61.953	2,7	169,3
TOTAL	-2.151.998	-2.316.919	100,0	107,7

FINAL RESULT	76.543	87.604	-	114,5

Prihodki Kemijskega inštituta

Revenues of the National Institute of Chemistry



SLIKA
Prihodki Kemijskega inštituta v mio EUR (povečanje za 57 % v obdobju 1999 - 2004).

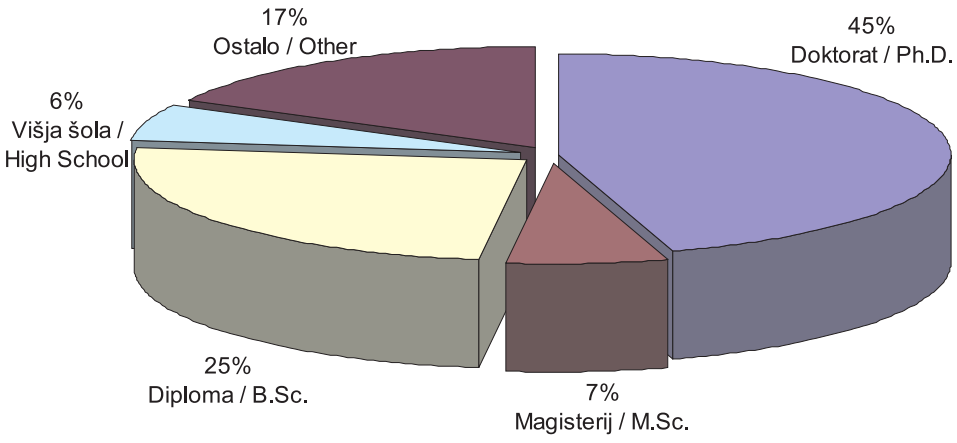
FIGURE
Revenues of the National Institute of Chemistry in million euros (57 % increase in the period 1999 - 2004).

Zaposleni

Personnel

Na dan 31. 12. 2004 je bilo na Kemijskem inštitutu 210 zaposlenih, od tega 95 doktorjev znanosti, 14 magistrov, 52 z visoko izobrazbo, 12 z višjo izobrazbo, 28 s srednjo in 9 z nižjo izobrazbo.

On December 31, 2004, we have recorded 210 employees with the following degree of education: Ph.D. (95), Master degree (14), Bachelor degree (52), Associate degree (12), secondary school (28) and less than secondary school (9).



SLIKA
Izobrazbena struktura zaposlenih na Kemijskem inštitutu v letu 2004.

FIGURE
Employees level of education at the National Institute of Chemistry in 2004.

Doktorati, magisteriji in diplome v letu 2004

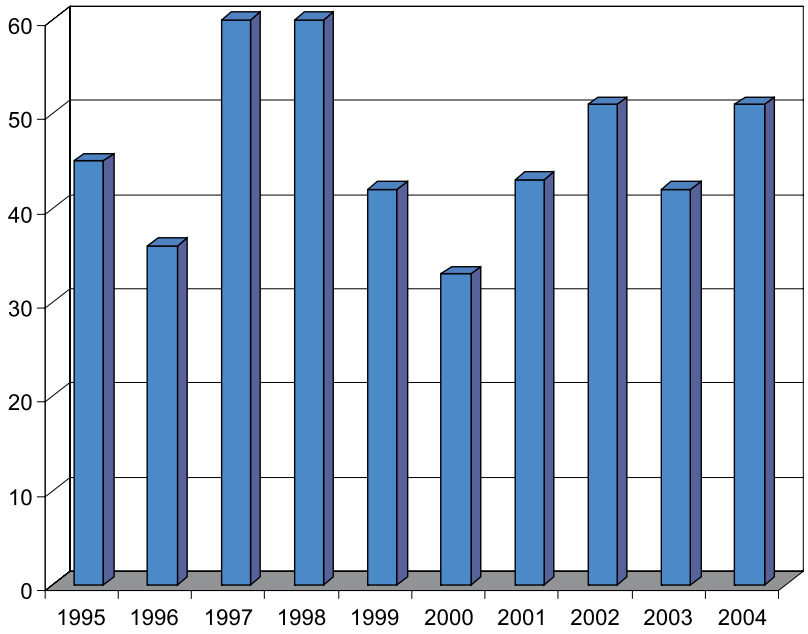
Doctoral, Master's and Graduate Theses in Year 2004

DOKTORATI / DOCTORAL THESES

- Mojca Štaudohar Kozjan, 13. 2. 2004
- Miroslav Kovačevič, 26. 3. 2004
- Samo Andrenšek, 4. 6. 2004
- Magda Cotman, 8. 7. 2004
- Gregor Mlinšek, 13. 9. 2004
- Ana Lenassi Zupan, 11. 10. 2004
- Marko Oblak, 3. 12. 2004
- Boštjan Podkrajšek, 20. 12. 2004

MAGISTERIJI / MASTER'S THESES

- Mateja Novak Štagoj, 22. 12. 2004



SLIKA
Doktorati, magisteriji in diplome v letih 1995 / 2004.

FIGURE
Ph.D., M.Sc., and B.Sc. theses in years 1995 / 2004.

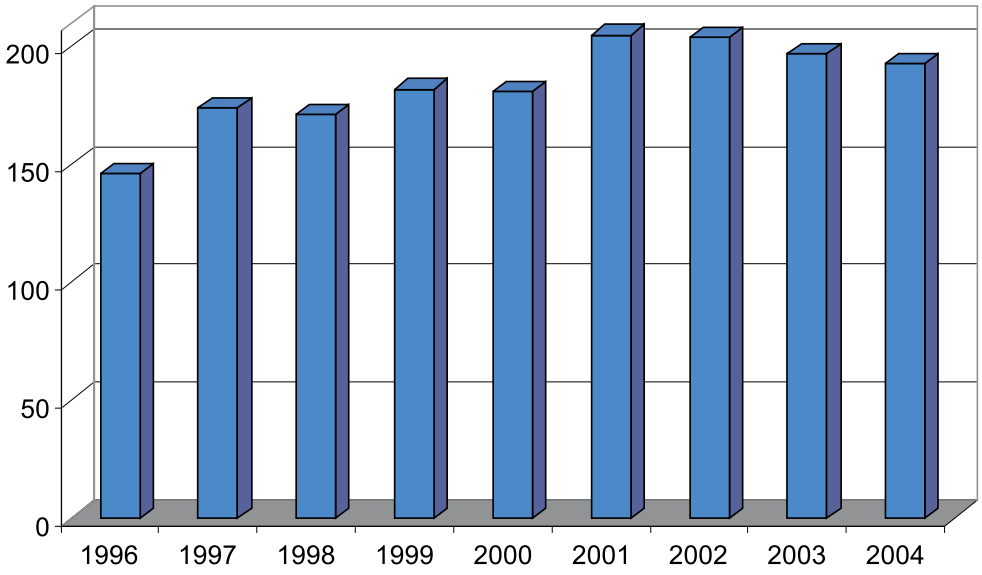
ŠTEVILO DIPLOM, MAGISTERIJEV, DOKTORATOV, MENTORSTEV IN KOMENTORSTEV S STRANI ZAPOSLENIH NA KI

NUMBER OF B. Sc., M. Sc., Ph. D. THESES, MENTORSHIPS AND COMENTORSHIPS BY EMPLOYEES OF NIC

3	diplomska dela / Graduate Theses
1	magistrsko delo / Master's Thesis
8	doktorskih disertacij / Doctoral Theses
13	mentorstev pri diplomskih delih / Mentorships of Graduation Theses
2	mentorstvi pri magistrskih delih / Mentorships of Master's Theses
6	mentorstev pri doktorskih disertacijah / Mentorships of Doctoral Theses
18	komentorstev pri diplomskih delih / Comentorships of Graduate Theses
2	komentorstvi pri magistrskih delih / Comentorships of Master's Theses
4	komentorstva pri doktorskih disertacijah / Comentorships of Doctoral Theses

Objave v letu 2004

Published Works in Year 2004



SLIKA
Objavljena dela (članki, knjige, poglavja, patenti) v letih 1996 / 2004.

FIGURE
Published works (papers, books, chapters, patents) in years 1996 / 2004.

Bibliografija inštituta v letu 2004
ANALITČNI PODATKI (tipologija COBISS / laboratoriji)

Institute bibliography for 2004
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	41	15	29	15	12	9	17	5	7	10	14	24	10	6	11	225	16	209
Prispevki na konferencah / Conference contributions	22	39	15	24	31	26	22	1	15	30	12	41	10	8	6	302	15	287
Patenti / Patents	0	1	0	0	1	2	4	3	0	1	5	1	1	0	0	19	0	19
Predavanja / Lectures	8	4	1	0	2	0	2	1	3	3	0	1	1	0	1	27	0	27
Dokumenti / Documents	1	0	0	7	20	0	3	0	0	2	0	2	2	14	1	52	2	50
Doktorati, magisteriji, diplome / PhD, MSc, BSc	6	3	1	2	8	2	2	1	1	2	8	9	0	5	1	51	0	51
SKUPAJ / ALL UNITS	**78**	**62**	**46**	**48**	**74**	**39**	**50**	**11**	**26**	**48**	**39**	**78**	**24**	**33**	**20**	**676**	**33**	**643**

Mednarodno sodelovanje

International Cooperation

MULTILATERALNO SODELOVANJE / MULTILATERAL COOPERATION	
5. Okvirni program EU / 5th Framework Programe EU	11
6. Okvirni program EU / 6th Framework Programe EU	5
COST	5
PROTEUS	3
Skupno / Total	**24**

BILATERALNO SODELOVANJE / BILATERAL COOPERATION	
Argentina / Argentina	1
Avstrija / Austria	1
Češka / Czech Republic	3
Francija / France	3
Grčija / Greece	3
Hrvaška / Croatia	6
Indija / India	2
Italija / Italy	6
Japonska / Japan	3
Madžarska / Hungary	2
Makedonija / Macedonia	1
Nemčija / Germany	1
Poljska / Poland	1
Portugalska / Portugal	1
Rusija / Russia	1
Srbija in Črna gora / Serbia and Montenegro	3
Turčija / Turkey	1
Velika Britanija / Great Britain	7
ZDA / USA	3
Skupno / Total	**49**

Nagrade podeljene sodelavcem inštituta v letu 2004

Awards Given To Collaborators with the Institute In 2004

Skladno s poslanstvom in vizijo o dolgoročnih ciljih Kemijskega inštituta, ki temeljijo tudi na motivaciji podiplomskih študentov, promociji Kemijskega inštituta na področju znanstveno-raziskovalnega dela in na izbiri in odlikovanju najboljših posameznikov, smo v letu 2004 na Kemijskem inštitutu prvič podelili:

Nagrado Kemijskega inštituta za izjemno doktorsko delo

Kandidirali so lahko vsi raziskovalci, ki so doktorirali v letih 2003 in 2004 in so opravili raziskovalno delo svoje dizertacije na Kemijskem inštitutu. Strokovna komisija, ki jo je imenoval Znanstveni svet Kemijskega inštituta je odločila, da se nagrada podeli dvema kandidatoma. Nagrado je podelil direktor inštituta, dr. Peter Venturini na novoletnem sprejemu Kemijskega inštituta, 9. 12. 2004. Nagrajenca sta:

- Dr. Matej Praprotnik; Nova simplektična metoda za simulacijo molekulske dinamike (mentor: dr. Dušanka Janežič)
- Dr. Gregor Mlinšek; Strukturno podprto načrtovanje trombinskih inhibitorjev (mentor: prof. dr. Tom Šolmajer)

In keeping with the mission and vision of the National Institute of Chemistry's (NIC) long - term goals, which are based on motivating post - graduate students, promoting the Institute in the area of scientific research, and honoring the best individuals, the Institute bestowed the following awards and recognitions for the first time in 2004:

The National Institute of Chemistry Award for Exceptional Doctoral Work

Candidates for this award are researchers who completed their doctoral research work at the National Institute of Chemistry in 2003 and 2004. A special commission named by the Scientific Council of NIC decided to grant the award to two candidates. The award was presented by the director of the Institute, Dr. Peter Venturini, at the Institute New Year's reception on December 9, 2004. The winners were:

- Dr. Matej Praprotnik; A New Simplectic Method for Simulating Molecular Dynamics (mentor: Dr. Dušanka Janežič)
- Dr. Gregor Mlinšek; Structurally Supported Design of Thrombin Inhibitors (mentor: Prof. Dr. Tom Šolmajer)

Vitez reda akademskih palm - visoko francosko odlikovanje, ki ga je podelila francoska veleposlanica v Sloveniji, gospa Dominique Gazuy 6. 5. 2004:
- Prof. dr. Radovan Komel

Zlati znak Jožefa Stefana, ki ga podeljuje Institut »Jožef Stefan« za najodmevnejša doktorska dela v Sloveniji v preteklih treh letih, 24. 3. 2004:
- Dr. Robert Dominko; Karakterizacija novih kompozitnih elektrod za litijeve ionske akumulatorje (mentor: doc. dr. J. Jamnik)

Zlato priznanje z listino – GZS, Območna zbornica Ljubljana za inovacijske dosežke v letu 2003 v ljubljanski regiji, 16. 11. 2004:
- Doc. dr. Matjaž Kunaver, prof.dr. Stanko Srčič, doc. dr. Odon Planinšek in Jernej Zadnik za inovacijo Razvoj metode za hitro in točno analizo površin praškov

34. Krkine nagrade 2004, Novo mesto, 29. 10. 2004:
- Janez Zupančič; Izolacija aktivne farmacevtske učinkovine iz sintezne mešanice s solventno ekstrakcijo (magistrska naloga, mentor: prof. dr. Viktor Grilc)
- Andrej Perdih; Kvantitativni odnos med strukturo in delovanjem (QSAR) peptidomimetikov s 3,4-dihidro-2H-1,4-benzooksazinskim skeletom (diplomska naloga, mentor: prof. dr. Tom Šolmajer)
- Alja Videtič; Preiskava mikrosatelitskih območij DNA pri raku želodca (diplomska naloga, mentor: prof. dr. Radovan Komel)
- Matjaž Vogelsang; Funkcijska analiza mutacije A92P človeškega gena MLH1 v kvasovki *Saccharomyces cerevisiae* (diplomska naloga, mentor: prof. dr. Radovan Komel)
- Janez Konc; Načrtovanje, sinteza in vrednotenje inhibitorjev rekombinantne 17β-hidroksisteroid dehidrogenaze iz glive *Cochliobolus lunatus* (raziskovalna naloga, mentor: prof. dr. Jurij Stojan)

Knight of the Order of Academic Palms – high - level French recognition granted by the French Embassy in Slovenia, Mrs. Dominique Gazuy, May 6, 2004:
- Prof. Dr. Radovan Komel

The Jožef Stefan Golden Emblem Prize, granted by the »Jožef Stefan« Institute for the most cutting edge doctoral work in Slovenia within the past three years, March 24, 2004:
- Dr. Robert Dominko; Characterization of New Composite Electrodes for Lithium Ion Accumulators (mentor: Dr. J. Jamnik, Assist. Prof.)

Golden Merit with Certificate – Chamber of Commerce of Slovenia, Regional Chamber for Ljubljana; Award for Innovative Achievements in 2003 in the Ljubljana region, November 16, 2004:
- Dr. Matjaž Kunaver, Assist. Prof., Prof. Dr. Stanko Srčič, Dr. Odon Planinšek, Assist. Prof. and Jernej Zadnik for innovation Development of Methods for Fast and Accurate Analysis of Surface Powders

34th Annual Krka Prizes, Novo Mesto, October 29, 2004:
- Janez Zupančič; Recovery of Active Pharmaceutical Ingredient from Reaction Mixture with Solvent Extraction (Master's Thesis, Mentor: Prof. Dr. Viktor Grilc)
- Andrej Perdih; Quantitative Structure Activity Relationship (QSAR) of Peptidomimetic Agents with a 3,4-Dihidro-2H-1,4-benzoxazine Scaffold (Undergraduate Thesis, Mentor: Prof. Dr. Tom Šolmajer)
- Alja Videtič; Study of Microsatellite DNA in Gastric Cancer (Undergraduate Thesis, Mentor: Prof. Dr. Radovan Komel)
- Matjaž Vogelsang; Functional Analysis of Human MLH1 Gene Mutation A92P in *Saccharomyces cerevisiae* (Undergraduate Thesis, Mentor: Prof. Dr. Radovan Komel)

Fakultetna Prešernova nagrada Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani za diplomsko delo, 1. 12. 2004:
- Petra Draškovič; Izolacija in karakterizacija rekombinantne mišje inozitolheksakisfosfatkinaze (mentor: prof. dr. Radovan Komel)

Fakultetna Prešernova nagrada Biotehniške fakultete Univerze v Ljubljani za diplomsko delo, 26. 11. 2004:
- Tanja Bagar; Priprava za pH občutljivega zeleno fluorescirajočega proteina, ki se izraža v glivi *Aspergillus niger* (mentor: prof. dr. Darja Žgur-Bertok, komentor: dr. Mojca Benčina)
- Janez Konc; Design, Synthesis and Evaluation of Inhibitors of Recombinant 17-β-Hydroxysteroid-Dehydrogenase from the Fungus *Cochliobolus lunatus* (Research Project, Mentor: Prof. Dr. Jurij Stojan)

Faculty Prešeren Prize presented by the Faculty of Chemistry and Chemical Technology of the University of Ljubljana for Undergraduate Thesis, December 1, 2004:
- Petra Draškovič; Isolation and Characterization of Recombinant Murine Inositol Hexakisphosphate Kinase (Mentor: Prof. Dr. Radovan Komel)

Faculty Prešeren Prize presented by the Biotechnical Faculty of the University of Ljubljana for Undergraduate Thesis, November 26, 2004:
- Tanja Bagar; Construction of a pH sensitive green fluorescent protein for expression in fungus *Aspergillus niger* (mentor: Prof. Dr. Darja Žgur-Bertok, comentor: Dr. Mojca Benčina)

L01

Laboratorij za molekularno modeliranje in NMR spektroskopijo

Laboratory for Molecular Modelling and NMR Spectroscopy

VODJA / HEAD
Prof. dr. Branko Borštnik

RAZISKOVALCI / RESEARCHERS
Dr. Franc Avbelj
Dr. Simona Golič Grdadolnik
Dr. Jože Grdadolnik
Dr. Milan Hodošček
Dr. Dušanka Janežič
Doc. dr. Janez Mavri
Dr. Franci Merzel
Prof. dr. Adolf Miklavc
Dr. Ksenija Poljanec
Dr. Matej Praprotnik
Dr. Danilo Pumpernik
Dr. Jernej Stare
Prof. dr. Tomaž Šolmajer

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Urban Borštnik
Urban Bren
Janez Konc
Gregor Mlinšek
Marko Oblak
Tjaša Urbič

TEHNIČNO OSEBJE / TECHNICAL STAFF
Tatjana Karba
Silva Zagorc

PRIPRAVNIKI / TRAINEES
Borut Tone Oblak

PODROČJA DEJAVNOSTI

Raziskovalni program P1-0010:

Folding in dinamika biomolekularnih sistemov (F. Avbelj)

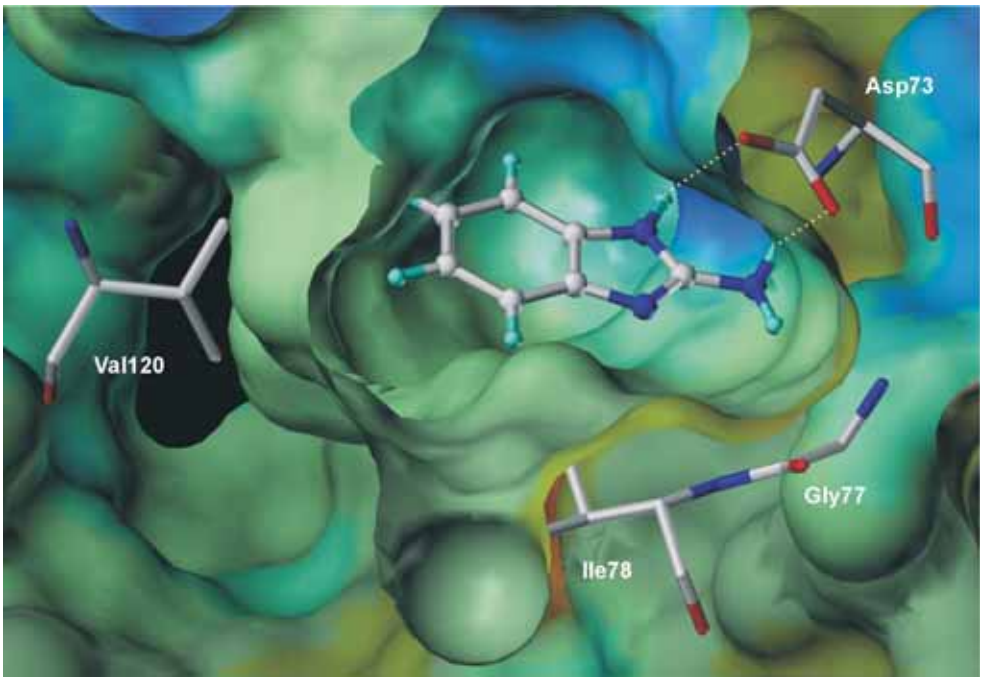
- Raziskave strukture in dinamike biomolekularnih sistemov (proteinov, ligandov, membran in njihovih kompleksov) z jedrsko magnetno resonanco, vibracijsko spektroskopijo in z računalniškimi simulacijami (Monte Carlo, molekulska dinamika)
- Študij elektrostatskih interakcij, vodikovih vezi, solvatacije (elektrostatsko senčenje) in hidrofobnih interakcij v proteinih, v sistemih ligand - receptor in v sistemih biomolekula - membrana

RESEARCH ACTIVITIES

Research program P0-501:

Protein folding and dynamics of biomolecular systems (F. Avbelj)

- 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



SLIKA

Sidranje 2-aminobenzimidazola v ATP-vezavno mesto proteina DNA giraze B. Proteinska okolica je predstavljena s topilu dostopno površino. Prikazani so tudi aminokislinski ostanki, ki so ključni za vezavo 2-aminobenzimidazola.

Model vezave je bil postavljen na osnovi dvodimenzionalnih 15N-HSQC eksperimentov izotopsko označenega proteina na NMR spektrometru Varian INOVA 600MHz v NMR centru.

FIGURE

Docking of 2-aminobenzimidazole in the ATP-binding site of the DNA gyrase B enzyme. Protein is presented as solvent accesible surface. Also shown are the amino acid residues that are critical for the binding of 2-aminobenzimidazole.

The model of binding was constructed by means of the two-dimensional 15N-HSQC experiments of the isotopically labeled protein on the NMR spectrometer Varian INOVA 600MHz in Slovenian NMR centre.

- 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 teotetskimi metodami
- Razvoj metod jedrske magnetne resonance za določanje konformacije molekul v tekočini
- Uporaba vibracijske spektroskopije in jedrske magnetne resonance v analizne namene

Raziskovalni program P1-0012:
Molekulske simulacije in bioinformatika (B. Borštnik)
- Kvantno kemijski izračuni strukturnih in elektronskih parametrov molekul in supramolekularnih sistemov
- Študij dinamike tvorbe in razpada medmolekulskih 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 in perkolacijski pojavi
- Racionalno načrtovanje novih zdravilnih učinkovin na osnovi strukture receptorja in proučevanja mehanizma inhibicije encimov

Raziskovalni program P1-0002:
Računalniško modeliranje strukture in dinamike molekul (D. Janežič)
Raziskovalni projekti:
J1-6331: Razvoj računalniških algoritmov za simulacije makromolekularnih sistemov (D. Janežič)

- 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 P0-502:
Molecular simulations and bioinformatics (B. Borštnik)
- Quantum chemical calculations of structural and electronic parameters of molecules and supramolecular systems
- Studies of dynamics of formation and decay of intermolecular bonds atom - transfer reactions
- Simulation of proton transfer reactions in hydrated systems using the methods of classical and quantum molecular simulations
- Study of endogeneous cancerogenesis
- Bioinformatics and study of biological evolution
- Statistical mechanics and percolation phenomena
- Structure - based drug design approach is used for mechanistic studies of enzyme inhibition and design of novel bioactive compounds

J1-5115: Simulacije in strukturna analiza vode ob površini proteinov (F. Merzel)
Z1-3036: Razvoj algoritmov za kombinirane kvantno / klasične simulacije (F. Merzel)

Razvoj in uporaba metod za molekularno modeliranje:

- Simplektične metode za simulacijo molekulske dinamike makromolekul
- Kombinacije metod simulacije molekulske dinamike, analize po normalnih načinih nihanja in kvaziharmonske analize proteinov v raztopinah za študij hidratacije proteinov
- Razvoj in uporaba QM/MM metod
- 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 gruče

BIBLIOGRAFIJA

27 izvirnih znanstvenih člankov
2 pregledna znanstvena članka
1 strokovni članek
1 samostojni znanstveni sestavek v monografiji
1 recenzija, prikaz knjige, kritika
1 predgovor, spremna beseda
1 drug članek ali sestavek
5 srednješolski, osnovnošolski ali drugi učbeniki z recenzijo
1 drugo učno gradivo
1 priročnik
1 objavljeni znanstveni prispevek na konferenci (vabljeno predavanje)
4 objavljeni znanstveni prispevki na konferencah
1 objavljeni strokovni prispevek na konferenci

Research program P1-0002:
Computer simulation of molecular structure and dynamics (D. Janežič)
Research projects:
J1-6331: Computer Algorithms Development for Macromolecular Simulation (D. Janežič)
J1-5115: Simulations and structural analysis of water at protein surfaces (F. Merzel)
Z1-3036: Algorithms development for combined classical/quantum simulations (F. Merzel)
Development and application of methods for molecular modeling:

- Symplectic methods for molecular dynamics simulations of macromolecules
- Combination of molecular dynamics methods, normal mode vibrational analysis, and quasiharmonic analysis of proteins in solutions for studying protein hydration
- Development and use of QM/MM methods
- Development of computationally efficient methods for determining the time - dependent electronic structure of molecules based on the Kohn - Sham formulation of the density functional theory
- Development and application of quantum chemical and classical approaches for calculating reaction mechanisms, especially calculating the ionic reactions of isocyanides
- Development and use of the RISM formalism
- Development of new and effective network topologies for connecting personal computers into clusters

BIBLIOGRAPHY

27 Original Scientific Articles
2 Review Articles
1 Professional Article
1 Scientific Article in a Monograph
1 Review, Book Review, Critique
1 Preface, Afterword
1 Other Article
5 Reviewed Secondary and Primary School Textbooks or Other Textbooks
1 Other Educational Material

15 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 objavljeni povzetek strokovnega prispevka na konferenci
3 predavanja na tujih univerzah
5 prispevkov na konferencah brez natisa
1 končno poročilo o rezultatih preiskav
2 diplomi
1 magisterij
3 doktorati
4 uredništva revij

GLAVNI DOSEŽKI V LETU 2004

- Novejše raziskave kažejo, da imajo denaturirani proteini strukturo, ki je do neke mere podobna strukturi nativne oblike. Ta struktura je zelo pomembna za razumevanje procesa zvitja proteinov ("protein folding"). Struktura denaturiranih proteinov se najbolj jasno pokaže v efektu najbližjega soseda ("the nearest - neighbor effect"), ki smo ga pojasnili s senčenjem elektrostatskih interakcij med atomi glavne verige.
- Odmiki kemijskih premikov HA, CA, in CB atomov od karakterističnih vrednosti naj bi bili zanesljivi kazalci sekundarnih struktur proteinov ("Chemical Shift Index method").
- Z analizo velikega števila kemijskih premikov v proteinih smo pokazali, da topilo močno vpliva na kemijske premike. Za nekatere amino kisline je vpliv topila na kemijske premike tako močan, da onemogoča določevanje sekundarnih struktur z NMR.

  Vpliv topila na kemijske premike je možno pojasniti le z elektrostatskim senčenjem, katerega pa uveljavljeni teoretski modeli kemijskih premikov ne upoštevajo.
- Na osnovi primerjalnih študij bioaktivnosti in konformacijskih lastnosti serije peptidnih in ne-peptidnih AT1 antagonistov smo načrtovali in sintetizirali novo spojino vodnico, ki je osnova za razvoj novih učinkovin za zdravljenje visokega krvnega pritiska. Konformacijske lastnosti smo določili z metodami NMR spektroskopije in molekularnega modeliranja.

1 Manual
1 Published Scientific Conference Contribution (Invited Lecture)
4 Published Scientific Conference Contributions
1 Published Professional Conference Contribution
15 Published Scientific Conference Contribution Abstracts
1 Published Professional Conference Contribution Abstract
3 Invited Lectures at Foreign Universities
5 Unpublished Conference Contributions
1 Final Research Report
2 Undergraduate Theses
1 Master's Thesis
3 Doctoral Dissertations
4 Editorships

IMPORTANT ACHIEVEMENTS IN 2004

- Denatured proteins in water have some residual structure that may be important in the folding process. The nature of the residual structure is currently of much interest. The residual structure is clearly demonstrated by a neighboring residue effect on backbone conformation. We have shown that the nearest - neighbor effect is caused by the screening of backbone electrostatic interactions by water dipoles.
- The chemical shift index method is commonly used to assign protein secondary structures. Analyzing a large number of chemical shifts we have shown that solvent strongly influences the chemical shifts of HA, CA, in CB atoms. The effect of solvent on the chemical shift of solvent exposed residues is so large that the conformational dependence of some residues disappears altogether, making identification of secondary structure by these shifts very difficult. We have shown that the solvent effect on chemical shifts can only be explained by the screening of backbone electrostatic interactions with solvent. This factor has been largely ignored.

- Z infrardečo in ramansko spektroskopijo smo raziskovali vpliv solvatacije na konformacijo proteinov. Pokazali smo, da so klasični pristopi določevanja sekundarne strukture proteinov nenatančni in v nekaterih primerih celo zavajajoči. Razvili smo novo metodo spektralne dekompozicije, ki nam omogoča vpogled v elementarne interakcije v biomolekulah. Tako smo lahko v proteinskem vibracijskem spektru razvrstili posamezna nihanja vodikovo vezanih skupin glede na jakost vodikove vezi.
- Raziskovali smo nekatere sisteme z zelo kratkimi inter - in intramolekularnimi vodikovimi vezmi, ki služijo kot modeli za strukturo in protonsko dinamiko v analognih povezavah na aktivnih mestih encimov. Pri tem uporabljamo metode, za katere ni eksperimentalnih možnosti na KI in se meritve opravljajo v sodelovanju z več laboratoriji po svetu. Zanimive rezultate smo že dobili na dihidratu oksalne kisline, monohidratih perfluorokarboksilnih kislin, na vrsti N-oksidov pikolinskih kislin in enolskih diketonih.
- Študirali smo H/D izotopske vplive na kemijske premike sistema z močno intramolekularno vodikovo vezjo. Eksperimentalno delo je bilo podprto z izračunanim spektrom. Pri izračunu smo poleg OH gibanja kvantizirali tudi OO koordinato in dobili odlično ujemanje z eksperimentom.
- Študirali smo alkilacijo gvanina v DNA z endogenimi končnimi karcinogeni s kvantno kemijskimi metodami. Za študij smo uporabili metode linearne zveze med prosto energijo aktivacije in reakcijsko prosto energijo.
- Z uporabo modelnih sistemov smo študirali del katalitične triade. Metode vibracijske spektroskopije smo kombiniranli s kvantno kemijskimi izračuni in reševanjem vibracijske Scroedingerjeve enačbe.
- Z metodo klasične molekulske dinamike smo študirali temperaturno odvisnost oblike signala povezanega z nihanjem kota OHO pri tekoči vodi. Pokazali smo, da je oblika signa-

- Comparison of bioactivity of a series of peptide and non - peptide AT1 antagonists with their conformational properties, which were determined by NMR spectroscopy and molecular modeling, led us to design and synthesis of a new leading compound for development of anti - hypertensive drugs. The molecule has a significant anti - hypertensive activity.
- We investigated the effects of solvation on protein conformation using infrared and Raman spectroscopy. We have shown that the classical methods of secondary structure determination are not adequate and sometimes even misleading. Therefore, we developed a method, which decomposes spectra to elementary ones. We have estimated the H-bond strengths of various protein groups.
- We examined some molecular systems with short inter - and intramolecular hydrogen bonds. These systems are used to study structure and proton dynamics in analogous enzyme active sites. We are using experimental techniques, which are not available at NIC. We have obtained some interesting results using the dihydrate of oxalic acid, monohydrate of perfluorocarboxy acids, a series of N-oxide-picolinic acids, and enol - diketones.
- Isotopic effects on chemical shift of a strong hydrogen bonded system was studied. Experimental work was combined with a two - dimensional quantum averaging. Beside OH cordinate also the OO coordinate was considered. Good agreement between the theory and experiment was reported.
- Alkylation of Gua by endogenous ultimate carcinogens was studied using quantum chemical methods. The linear free energy relationship was used to determine chemical reactivity.
- Part of the catalytic triad in serine proteases was studied by using model compounds. Quantum chemical calculations were combined by solving the vibrational Scroedinger equation and vibrational spectroscopy.

la povezana s poljem sile in ne s kvantno naravo gibanja jeder.

- Oblikovali smo modele vezavnih mehanizmov med receptorjem in ligandom v bioloških sistemih v pretežno hidrofobnem okolju s steričnimi omejitvami in pozitivno spremembo entropije. Dosedanje razlage mehanizmov niso popolnoma pojasnile eksperimentalnih podatkov. Kot možni model smo predlagali entropijsko zajetje. Model smo utemeljili s štirimi zgledi: z vezavo ligandov na GPCR, alkoholno in oktopin dehidrogenazo ter CaATP-azo.
- Z metodo proteinske kristalografije smo določili strukturo tripeptidomimetikov - inhibitorjev trombina z azafenilalaninskim fragmentom na mestu P2 in s heterobicikličnim fragmentom 4,5,6,7-tetrahidro-1,3-benzotiazolom na mestu P1, ki nadomeščata aminokisline v spojini vodnici D-Phe-Pro-Arg.
- Razvili smo novo metodo za oceno vezavne konstante inhibitorja na osnovi kvantno kemijskega deskriptorja molekularnega elektrostatskega potenciala in kemometričnega modela nevronskih mrež s povratno zanko (CP-ANN) in genetskega algoritma (skupaj s sodelavci iz L03).
- Razvili smo kvantitativne korelacije med strukturo in aktivnostjo za serijo alfa1-adrenergičnih antagonistov z uporabo nevronske mreže s povratno zanko (CP-ANN) in določili strukturne determinante njihove selektivnosti na podtipe adrenergičnih receptorjev 1a, 1b in 1c (skupaj s sodelavci L03 in Fakultete za farmacijo Univerze v Beogradu).
- Razvili smo kvantitativne korelacije med strukturo in aktivnostjo za serijo zaviralcev MurD ligaz, ki so pomembna tarča za razvoj antiinfektivnih učinkovin.
- Pripravili smo novo metodo za indirektno ovrednotenje podobnosti molekulskih oblik (skupaj z raziskovalci Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani).

- Temperature dependece of the HOH bending band in bulk water was studied using classical MD in conjunction with flexible SPC model. It was demonstrated that the anomalous temperature behaviour can be attributed to the water model rather than nuclear quantum effects.
- The ligand binding mechanisms to receptors were proposed for the cases with steric hindrances, hydrophobic environment and positive entropy changes. The existing models did not satisfactorily reproduce the experimental data. We proposed the mechanism of entropic trapping and presented four examples where the mechanism seems to be operative.
- Using protein crystallography we determined the structure of tripeptidomimetics -thrombin inhibitors with azaphenylalanine fragments in position P2, and incorporating heterobicyclic fragment 4,5,6,7-tetrahidro-1,3-benzotiazole in position P1, mimicking the amino acids in the lead compound D-Phe-Pro-Arg.
- A novel method for prediction of the inhibitors binding constant based on quantum - chemical descriptor molecular electrostatic potential and chemometric model of counterpropagation neural networks (CP-ANN) and genetic algorithm (in collaboration with L03).
- Quantitative structure - activity relationships for a series of alpha1 adrenergic antagonists were developed by using counterpropagation artificial neural nets and structural determinants of their selectivity towards adrenergic receptors subtypes 1a, 1b and 1c were determined (in collaboration with L03 and Faculty of Pharmacy, University of Belgrade, Serbia and Montenegro).
- Quantitative structure – activity relationships for a series of MurD ligase inhibitors were developed, which are an important target for antiinfective compounds.

- Na področju raziskave človeškega genoma smo nadaljevali s študijem mehanizmov zdrsov polimeraze. Analizirali smo podatkovno bazo enonukleotidnih polimorfizmov in tako pridobili nove podatke o mehanizmih, ki povzročajo raznolikost genetskega materijala.
- Z uporabo nove simplektične metode (SISM) za simulacijo molekulske dinamike smo študirali temperaturno odvisnost vibracijskega spektra vode. Ugotovili smo, da eksperimentalno ugotovljenega ožanja traku upogiba z naraščanjem temperature MD ne reproducira. Smo pa s tem pristopom uspešno reproducirali vse ostale eksperimentalno ugotovljene spektroskopske lastnosti vode.
- S pomočjo računalniških simulacij smo obravnavali termodinamske lastnosti vode, ki je v neposrednem stiku s proteini, pri čemer je bil glavni poudarek na strukturnih spremembah vode na površini proteinov in vlogi vode pri dinamskem prehodu v proteinu.
- Izpeljali smo proceduro za kolektivno komunikacijo na vzporednih računalniških sistemih sestalvljenih iz gruč osebnih računalnikov s pomočjo katere lahko znatno pospešimo izvajanje simulacije molekulske dinamike.
- S pomočjo resonančne teorije, ki sloni na dejstvu, da imata dve aromatični izomeri lahko različno število Kekulejevih struktur in da je izomera z večjim številom Kekulejevih struktur bolj stabilna, smo obravnavali aromatičnost nanocevk.
- Dr. Dušanka Janežič je Associate Editor revije Journal of Chemical Information and Modeling (prej Journal of Chemical Information and Computer Sciences), American Chemical Society Publications. Uredila je posebno številko JCICS-a posvečeno dr. George W. A. Milne-ju za njegovo 20 - letno editorsko delo.
- Dr. Milan Hodošček je soavtor in razvijalec najbolj uporabljanega računalniškega programa za molekularno modeliranje - CHARMM (Chemistry at HARvard Molecular Mechanics).
- A novel method for indirect evaluation of molecular shape similarity was developed (in collaboration with researchers of Faculty for Chemistry and Chemical Technology, University of Ljubljana, Slovenia).
- In the field of study of human genome the polymerase slippage mechanisms were further scrutinized by the analyses of single polymorphism database. New insight was obtained regarding the details of the slippage process.
- Temperature dependence of water vibrational spectrum was studied by SISM, a newly developed molecular dynamics simulation method. The experimentally determined narrowing of the bending band with increasing temperature is not reproducible by MD simulation. However, this approach successfully reproduces all other experimentally observed properties of bulk water.
- Using computer simulations of solvated proteins, we studied the thermodynamics of internal and surface water molecules. The emphasis was on the modification of average solvent structure on a protein surface, the role of water in the protein dynamical "glass" transition and a simplified description of the protein motions thereby activated.
- A procedure was derived to obtain a performance gain for molecular dynamics simulations on existing parallel clusters.
- The resonance energy of carbon nanotubes and nanoribons was determined by enumerating the conjugated circuits and Kekule structures.
- Dr. Dušanka Janežič is an Associate Editor of the Journal of Chemical Information Modeling (formerly Journal of Chemical Information and Computer Sciences), American Chemical Society Publications. She edited a special issue of JCICS dedicated to Dr. George W.A. Milne for his long dedicated service as the Editor - in - Chief of JCICS.
- Dr. Milan Hodošček is a coauthor and developer of the widely used computer program

- Dr. Matej Praprotnik je prejel nagrado Kemijskega inštituta za izjemno dokotrsko delo.
- Janez Konc je prejel Krkino nagrado za raziskovalno nalogo.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V sodelovanju s firmo Lek d.d., Ljubljana; raziskave učinkovin delamo na projektih raziskav novih učinkovin na kardiovaskularnem in antiinfektivnem terapevtskem področju.

MEDNARODNO SODELOVANJE

- Dr. Thomas Mavromoustakos, Institute of Organic and Pharmaceutical Chemistry, The National Hellenic Research Foundation, Atene, Grčija: Slovensko - grški projekt (BI-GR/02-05-007) Conformational analysis and drug - membrane interactions of bioactive compounds; slovenski nosilec: dr. Simona Golič Grdadolnik
- Slovensko - poljski bilateralni projekt (BI-PL/04-05-001), "Self - organization of bilayer membranes constituted from phenolic lipids and derivatives of phenolic lipids. An experimental and theoretical study." Faculty of Chemistry, University of Wroclaw; Poljska; nosilca: dr. Jože Grdadolnik, prof. Alexander Koll
- Sodelujemo na mednarodnih projektih NATO Collaborative Linkage Grant in COST D23, katerih odgovorni nosilec je dr. Milan Hodošček
- 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

  z Rusijo: dr. Vladimir V. Poroykov, Institute of Biomedical Chemistry of Russian Academy of Medical Sciences, Moscow, Rusija

  s Francijo: dr. Alain Sanson, CEA, Saclay, Pariz, Francija

for molecular modeling - CHARMM (Chemistry at HARvard Molecular Mechanics).

- Dr. Matej Praprotnik received a National Institute of Chemistry award for outstanding doctoral work.
- Janez Konc received a Krka award for a research project.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

In collaboration with Lek d.d., Ljubljana, Slovenia, a new Sandoz company - Drug Discovery we develop novel chemical entities (NCE's) in the antiinfective and cardiovascular therapeutic areas.

INTERNATIONAL COLLABORATION

- Dr. Thomas Mavromoustakos, Institute of Organic and Pharmaceutical Chemistry, The National Hellenic Research Foundation, Athens, Greece: Slovenian - Greek project (BI-GR/02-05-007) Conformational analysis and drug - membrane interactions of bioactive compounds; slovenian project leader: Dr. Simona Golič Grdadolnik
- Slovenian - Polish project (BI-PL/04-05-001), "Self - organization of bilayer membranes constituted from phenolic lipids and derivatives of phenolic lipids. An experimental and theoretical study." Faculty of Chemistry, University of Wroclaw; Poland; project leaders: Dr. Jože Grdadolnik, Prof. Alexander Koll
- We are collaborators of the international NATO projects Collaborative Linkage Grant and COST D23 (Dr. Milan Hodošček)
- 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

  Russia, Dr. Vladimir V. Poroykov, Institute of Biomedical Chemistry of Russian Academy of Medical Sciences, Moscow, Russia

z Nemčijo: dr. Jeremy C. Smith, IWR Biocomputing, University of Heidelberg, Heidelberg, Nemčija

z Japonsko: dr. Tetsu Nurumi, RIKEN Institut, Jokohama, Japonska

s Hrvaško: dr. Sonja Nikolić, Institut Rudjer Bošković, Zagreb, Hrvaška

s Hrvaško: dr. Sanja Tomić, Institut Rudjer Bošković, Zagreb, Hrvaška

s Turčijo: dr. Gamze Tanoglu, Izmir Institute of Technology, Izmir, Turčija

z Madžarsko: dr. Istvan Lukovits, Chemical Research Center, Hungarian Academy of Sciences, Budapest, Madžarska (medakademijski projekt)

POMEMBNI INŠTRUMENTI IN OPREMA

- NMR spektrometri v okviru Slovenskega NMR centra
- FTIR spectrometer Bruker IFS 66S
- PE 2000 NIR Ramanski spektrometer
- Računalniška oprema: SG delovne postaje, paralelni računalniški sistemi VRANA, sestavljeni iz 200 Athlon procesorjev

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Mlinšek Gregor; Strukturno podprto načrtovanje trombinskih inhibitorjev, doktorska disertacija, Ljubljana 2004 (mentor: T. Šolmajer)
- Oblak Marko; Strukturno podprto načrtovanje novih inhibitorjev DNA giraz z delovanjem na ATP-vezavnem mestu: doktorska disertacija, Ljubljana: 2004 (mentor: T. Šolmajer)
- Erić Slavica; Molekulsko modeliranje i korelacija kvantitativnih odnosa strukture, dejstva i selektivnosti alfa1-adrenergičkih antagonista : doktorska disertacija, Beograd 2004 (komentor: T. Šolmajer)
- Perdih Andrej; Kvantitativni odnos med strukturo in delovanjem (QSAR) peptidomimetikov s 3,4-dihidro-2H-1,4-benzooksazinskim

France, Dr. Alain Sanson, CEA, Saclay, Paris, France

Germany, Dr. Jeremy C. Smith, IWR Biocomputing, University of Heidelberg, Heidelberg, Germany

Spain, Dr. Marie Paz Calvo, University of Valliadolid, Valliadolid, Spain

Japan, Dr. Tetsu Nurumi, RIKEN Institute, Jokohama, Japan

Croatia, Dr. Sonja Nikolić, Institute Rudjer Bošković, Zagreb, Croatia

Croatia, Dr. Sanja Tomić, Institute Rudjer Bošković, Zagreb, Croatia

Turkey, Dr. Gamze Tanoglu, Izmir Institute of Technology, Izmir, Turkey

Hungary, Dr. Istvan Lukovits, Chemical Research Center, Hungarian Academy of Sciences, Budapest, Hungary

EDUCATION AND IMPORTANT VISITS

- Mlinšek Gregor; Structure based design of thrombin inhibitors – Ph.D. Thesis, Ljubljana 2004 (supervisor: T. Šolmajer)
- Oblak Marko; Structure based drug design of novel ATPase inhibitors of the DNA gyrase – Ph.D. Thesis, Ljubljana, 2004 (supervisor: T. Šolmajer)
- Erić Slavica; Molecular modeling and QSAR including selectivity of alpha1-adrenergic antagonists : Ph.D. thesis Belgrade, 2004. (co - supervisor: T. Šolmajer)
- Perdih Andrej; Quantitative structure activity relationsip (QSAR) of peptidomimetic agents with 3,4-dihidro-2H-1,4-benzooxazine scaffold - B.Sc. thesis, Ljubljana, 2004 (co - supervisor: T. Šolmajer)
- Dr. Dušanka Janežič was promoted to the position of Research Professor at the University of Ljubljana, Slovenia
- Urban Borštnik was granted a direct transfer to the doctoral degree under the advisorship of Dr. Dušanka Janežič

skeletom; diplomsko delo, Ljubljana, 2004 (komentor: T. Šolmajer)

- Dr. Dušanka Janežič je bila na Univerzi v Ljubljani izvoljena v naziv znanstvene svetnice
- Urbanu Borštniku je bil pod mentorskim vodstvom dr. Dušanke Janežič odobren neposredni prehod na doktorski študij

L02

Laboratorij za spektroskopijo materialov

Laboratory for Spectroscopy of Materials

VODJA / HEAD
Prof. dr. Boris Orel

RAZISKOVALCI / RESEARCHERS
Dr. Zorica Crnjak Orel
Dr. Marta Klanjšek Gunde
Dr. Angela Šurca Vuk
Dr. Urška Lavrenčič Štangar (do / until 7. 11. 2004)
Dr. Lidija Slemenik Perše (od / since 8. 11. 2004)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Robi Ješe
Jelica Vince
Vasko Jovanovski
Mojca Fir

TEHNIČNO OSEBJE / TECHNICAL STAFF
Miljana Horvatić
Helena Spreizer

PODROČJA DEJAVNOSTI

- Razvoj materialov za fotoelektrokemične celice (nanokristalinični TiO_2 filmi, redoks elektroliti na osnovi ionskih tekočin)
- Razvoj selektivnih premazov za sončne zbiralnike (v okviru Solabs EU projekta in kot samostoji projekt za MORS)
- Razvoj nanokompozitnih filmov za korozijsko zaščito kovin (v okviru Solabs in kot samostojni projekt v letu 2004)
- Razvoj metod za študij optičnih in strukturnih lastnost pigmentih disperzij (v sodelovanju s Colorjem)
- Raziskave porazdelitve in velikosti nanodelcev s pomočjo spektroskopskh metod (pretežno interkalacijskih spojin za elektrokromne sklope)
- Barve in barvna metrika

RESEARCH ACTIVITIES

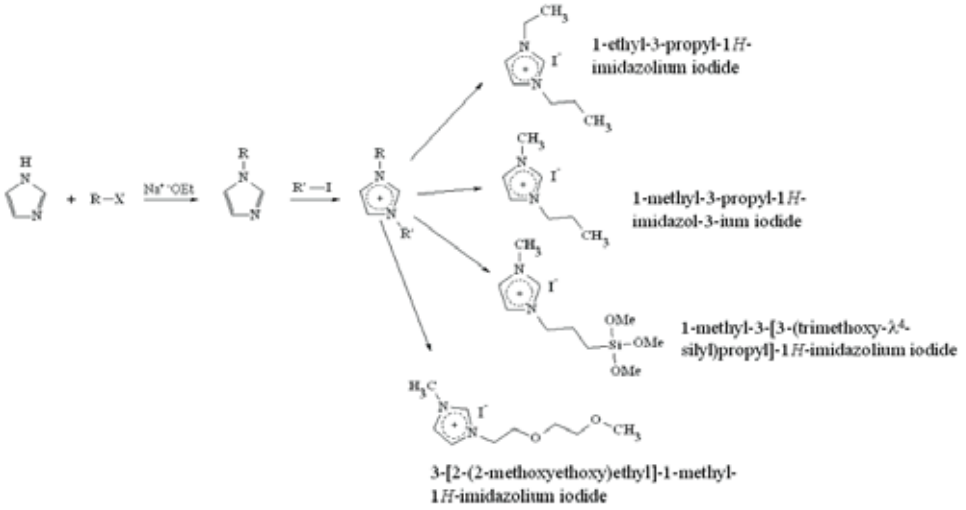
- Development of materials for photoelectrochemical cells (nanocrystalline TiO_2 films, redox electrolytes on the basis of ionic liquids)
- Development of selective coatings for solar absorbers (Solabs EU project, MORS project)
- Development of nanocomposite films for corrosion protection of metals (Solabs EU project, project MVŠZT)
- Development of methods for the study of optical and structural properties of pigment dispersions (in cooperation with Color d.d., Medvode, Slovenia)
- Investigation of nanoparticles with regard to their size using various spectroscopic methods (mainly intercalation compounds for electrochromic devices)
- Colours and colour metrics

BIBLIOGRAFIJA

12 izvirnih znanstvenih člankov
3 samostojni znanstveni sestavki v monografijah
8 objavljenih znanstvenih prispevkov na konferencah

BIBLIOGRAPHY

12 Original Scientific Articles
3 Scientific Articles in Monographs
8 Published Scientific Conference Contributions



SLIKA

Sintezne poti različnih ionskih tekočin.

FIGURE

Synthesis routes of various ionic liquids

5 objavljenih strokovnih prispevkov na konferencah
25 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 objavljeni povzetek strokovnega prispevka na konferenci
1 patentna prijava
3 predavanja na tujih univerzah
1 prispevek na konferenci brez natisa
1 diploma
1 magisterij
1 doktorat

5 Published Professional Conference Contributions
25 Published Scientific Conference Contribution Abstracts
1 Published Professional Conference Contribution Abstract
1 Patent Application
3 Invited Lectures at Foreign Universities
1 Unpublished Conference Contribution
1 Undergraduate Thesis
1 Master's Thesis
1 Doctoral Dissertation

GLAVNI DOSEŽKI V LETU 2004

- V preteklem letu smo iskali nove eksperimentalne in analizne pristope in se usmerili na sintezo novih materialov. Poleg tega je bilo preteklo leto ključno za raziskave, ki so potekale v okviru Solabs EU projekta. Premazi, narejeni v letu 2004, bodo služili za pripravo kolektorjev in sončnih fasad, na njih bodo v tekočem letu preostali parnerji preverili uporabnost v realnih sistemih. Bistven rezultat raziskav premazov - opravili smo jih v tesnem sodelavanju s podjetjem Color d.d., Medvode - so barve, ki preprečujejo ohlajevanje segrete površine v kolektorju tako, da znižajo njegove radiacijske izgube. To smo dosegli tako, da smo v pigmentne mešanice vmešali kovinske pigmente (površinsko obdelan aluminj). Merilo za doseženi clij je razmerje med deležem sončnega sevanja, ki ga površina premaza absorbira (sončna absorptivnost α_s) in deležem infrardečega, t.j. toplotnega sevanja, ki ga površina emitira (termična emisivnost ε_T). Tipične vrednosti za črne premaze so α_s = 0.90 - 0.92 in ε_T = 0.38 - 0.42. Premazi z drugačnimi niansami (temno modra, rdeča in zelena niansa) - to je bil glavni namen Solabs projekta - pa dosežejo α_s = 0.85 - 0.89 ter ε_T = 0.38 - 0.34. Premazi so razviti že do komercialne faze, povpraševanje se že kaže in pričakujemo, da bo naše delo imelo neposredni finančni učinek.
- Pridobili smo nov projekt, ki ga financira MORS, v sklopu katerega moramo narediti

IMPORTANT ACHIEVEMENTS IN 2004

- In the previous year we searched for new experimental and analytical approaches and were devoted to the synthesis of new materials. Year 2004 was also crucial for the investigations in the frame of Solabs EU project. We prepared paint coatings for solar collectors and facades that will be tested during this year by other Solabs partners in real systems. The paint coatings - prepared in cooperation with the factory Color d.d., Medvode, Slovenia - prevent cooling of the heated collector area by decreasing its radiation losses. This was achieved by incorporation of metal pigments (coated aluminium flakes) in paints and reflects in ratio of solar radiation absorbed by the coated area (solar absorptance α_s) and infrared, i.e. heat, radiation emitted (thermal emittance ε_T). Typical values of black coatings are α_s = 0.90 - 0.92 and ε_T = 0.38 - 0.42. Coatings with dark blue, red and green colours - this was the main objective of Solabs project - attain α_s = 0.85 - 0.89 and ε_T = 0.38 - 0.34. Paint coatings have already been developed up to commercial phase.
- In the frame of new project, financed by MORS, we develop coatings with small observance for termovision observation. The project includes also Fotona d.d., Ljubljana, Slovenia; University in Maribor, Slovenia and Color d.d., Medvode, Slovenia.

premaze, ki imajo majhno opaznost za termovizijsko opazovanje. Projekt vključuje še Fotono d.d., Ljubljana, Univerzo v Mariboru in Color d.d., Medvode.

- Naslednji projekt, ki smo ga pridobili od MVŠZT, se nanaša na nanokompozitne filme za zaščito kovin. Tematika je nova, vendar se je pokazalo, da lahko koristno uporabimo izkušnje o sol-gel kemijskih postopkih, merjenju lastnosti solov in gelov s spektroskopskimi metodami in poznavanju sinteze sol-gel nanokompozitov. Ta projekt nam je omogočil, da smo pospešili tudi delo v okviru Solabs projekta, in sicer pri pripravi zaščitnih filmov za tankoslojne absorberje, ki jih dela nemško podjetje Interpane. Rezultati so vzpodbudni.
- Med najpomembnejše dosežke sodi priprava novih ionskih tekočin, ki se lahko kot redoks elektroliti uporabljajo v Graetzlovih fotoelektrokemijskih celicah. V laboratoriju smo pripravili ionsko tekočino, ki vsebuje reaktivne trialkoksisilanske skupine. Pri pogojih kislinske katalize te med seboj reagirajo, viskoznost se poveča, nastali material ne teče več in doseže kvazi trdno stanje. Ker ionske tekočine niso hlapne, že preprosto tesnenje zadošča za pripravo Graetzlovih celic.
- Raziskali smo vpliv, ki ga imajo sestavine in proizvodni parametri pri pripravi premaznega prahu na videz utrjenega praškastega premaza (PC). Zaključili smo analizo efektnih PC in matiranja neefektnih PC. Analizirali smo lastnosti selektivnega jedkanja s kisikovo plazmo na nekaj različnih polimerih, ki se uporabljajo pri mokrih pigmentiranih premazih.
- Svetlobo v prostoru s preklopnimi okni smo analizirali s standardnimi metodami za barvni videz svetlobe. Izkazalo se je, da nobena od teh metod ne more zadovoljivo opisati fenomena, zato smo rezultate prikazali v 3D barvnem prostoru CIELAB. Z obarvanjem preklopnega okna pride do izrazito nelinearne transformacije barvnega prostora. Napove-

- Next project, financed by the Ministry of Higher Education, Science and Technology of the Republic of Slovenia refers to nanocomposite films for protection of metals. Our knowledge about the sol-gel chemical procedures, synthesis of sol-gel nanocomposites and measurements of the properties of sols and gels using various spectroscopic methods were quite beneficial for the start of this project. This project enabled us also to accelerate the work in the part of Solabs project engaged with the protective films for thin - layered absorbers produced by German factory Interpane. The results are encouraging.
- Among our most important achievements we count the synthesis of new ionic liquids that can be used as redox electrolytes in Graetzel photoelectrochemical cells. In the laboratory we synthesised an ionic liquid that contains reactive trialkoxysilane groups. In the conditions of acid catalysis these groups interact, viscosity increases; the new material reaches the quasi-solid state. Ionic liquids are not volatile therefore their leakage is not problematic for the lamination of Graetzel cells.
- We investigated the influence of the compounds and production parameters on the preparation of coating powder and visual appearance of cured powder coating (PC). We finalized the analysis of the optical properties of effect PC and the matting process of non - effect PC. We analysed the selective oxygen plasma etching of various polymers that can be used as a binder in pigment coatings.
- Lighting in the room with switchable windows was analysed by standard methods for colour rendering of light. It was found that standard methods could not satisfactorily describe the phenomenon, therefore the results were shown in 3D colour space CIELAB. Coloration of the switchable window leads to a non - linear transformation of the colour space. The colorimetrically predicted changes were confirmed by measurements.

dane barvnometrične spremembe svetlobe smo potrdili tudi z merjenji.

- S pomočjo GISAXS in GIXR meritev (ELETTRA sinhrotron, Trst, Italija) smo ugotavljali možne spremembe v velikosti delčkov in poroznosti v vanadijevem oksidu in V/Ce oksidih, pripravljenih pri 38 in 55 at.% V po interkalaciji Li^+ ionov. Ugotovili smo, da se po interkalaciji Li^+ ionov povprečna velikost delčkov, dobljenih z GISAXS meritvami, spreminja po debelini nanosa. Tako se povprečna velikost delčkov za vzorce vanadijevega oksida po inerkalaciji Li^+ ionov zmanjšuje, za vzorce V/Ce oksida, pripravljenih pri 38 in 55 at.% V, pa povečuje. Poroznost se zmanjšuje v vzorcih, pripravljenih z 38 in 55 at.%.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Color d.d., Medvode; razvoj premazov za absorberje sončnih zbiralnikov za fasade - sodelovanje v okviru EU projekta Solabs
- Helios d.d., Domžale; licenčna pogodba

MEDNARODNO SODELOVANJE

- Solabs, Development of unglazed solar absorbers for building facades, and integration into heating systems (ENK6-CT-2002-00679), EU projekt, 6. okvirni program (B. Orel)
- Nanostructured and Functional Polymer - Based Materials and Nanocomposites, Proposal No. NOE 500361-2, Mreža odličnosti (Z. Crnjak Orel)
- Coordinated research project IAEA, IAEA-TECDOC, 1409 (M. Klanjšek Gunde)
- CIE, Division 1 (M. Klanjšek Gunde, uradna članica)
- CIE, Division 2, TC2-53 Multi - geometry color measurements of effect materials (M. Klanjšek Gunde, članica)
- Raziskave neurejenih materialov: Nano optični nanosi, Bilateralno sodelovanje Slovenija - Hrvaška (Institut Rudjer Bošković, Zagreb, Hrvaška), (Z. Crnjak Orel)

- Using GISAXS and GIXR measurements (ELETTRA synchroton, Trieste, Italy) we studied possible changes in the size of particles and porosity in vanadium oxide and V/Ce oxides thin films prepared at 38 and 55 at.% V after intercalation of Li^+ ions. We found out that the average size of the particles, obtained by GISAXS, after intercalation of Li^+ ions changed accros the layer: it decreased for vanadium oxide, but increased for V/Ce samples prepared at 38 in 55 at.% V. The porosity diminished in samples prepared at 38 and 55 at.%.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Color d.d., Medvode, Slovenia; development of coatings for solar absorber facades; cooperation in the frame of Solabs EU project
- Helios d.d., Domžale, Slovenia; licence agreement

INTERNATIONAL COLLABORATION

- Solabs, Development of unglazed solar absorbers for building facades, and integration into heating systems (ENK6-CT-2002-00679), EU project, 6th frame (B. Orel)
- Nanostructured and Functional Polymer - Based Materials and Nanocomposites, Proposal No. NOE 500361-2, Network of excellence (Z. Crnjak Orel)
- Coordinated research project IAEA, IAEA-TECDOC, 1409 (M. Klanjšek Gunde)
- CIE, Division 1 (M. Klanjšek Gunde)
- CIE, Division 2, TC2-53 Multi - geometry colour measurements of effect materials (M. Klanjšek Gunde)
- Investigations of disordered materials: Nanooptical coatings, Bilateral cooperation Slovenia - Croatia (Institut Rudjer Bošković, Zagreb, Croatia), (Z. Crnjak Orel)
- Preparation and characterisation of uniform particles, Bilateral cooperation Slovenia - USA (Clarkson University, Potsdam, New York, USA), (Z. Crnjak Orel)

- Priprava in karakterizacija uniformnih delcev, Bilateralno sodelovanje Slovenija - ZDA (Clarkson University, Potsdam, New York, ZDA), (Z. Crnjak Orel)
- Nanoporozni sol-gel materiali za elektrokromne aplikacije, Bilateralno sodelovanje Slovenija - Italija (Universita di Roma "La Sapienza", Italija), (A. Šurca Vuk)
- Nanokompozitni organsko / anorganski ionski prevodniki in njihova uporaba v fotoelektrokemijskih sončnih celicah, Bilateralno sodelovanje Slovenija - Grčija (Univerza v Patrasu, Grčija), (B. Orel)

POMEMBNI INŠTRUMENTI IN OPREMA
- FT-IR spektrometer Bruker IFS 66/S
- FT-IR in FT-Raman spektrometer Perkin Elmer 2000
- Hewlett-Packard 8453 UV-VIS spektrofotometer z diodnim nizom
- AUTOLAB PGSTAT30 in EG&G PAR 273 potenciostat/galvanostat

IZOBRAŽEVANJE
Mentorstva:
- Robi Ješe, Jelica Vince in Mojca Fir (mentor B. Orel), Vasko Jovanovski (mentor A. Šurca Vuk)
- Aljaž Vilčnik in Boštjan Japelj (komentor B. Orel)
- Mojca Vrčon (diplomsko delo, komentor Z. Crnjak Orel)
- Daša Šivec (praktikantka, mentor B. Orel)

- Nanoporous sol-gel materials for electrochromic application, Bilateral cooperation Slovenia - Italy (Universita di Roma "La Sapienza", Italy), (A. Šurca Vuk)
- Study of nanocomposite organic/inorganic conductors and their applications to photoelectrochemical solar cells, Bilateral cooperation Slovenia - Greece (University of Patras, Greece), (B. Orel).

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

EDUCATION AND IMPORTANT VISITS
Mentorships:
- Robi Ješe, Jelica Vince in Mojca Fir (mentor B. Orel), Vasko Jovanovski (mentor A. Šurca Vuk)
- Aljaž Vilčnik in Boštjan Japelj (comentor B. Orel)
- Mojca Vrčon (diploma work, comentor Z. Crnjak Orel)
- Daša Šivec (practical lab work, mentor B. Orel)

L03

Laboratorij za kemometrijo

Laboratory of Chemometrics

VODJA / HEAD
Prof. dr. Jure Zupan (do / until 5. 12. 2004)
Dr. Marjana Novič, v.d. (od / since 6. 12. 2004)

RAZISKOVALCI / RESEARCHERS
Dr. Marjana Novič (do / until 5. 12. 2004)
Dr. Marjan Vračko
Dr. Neva Grošelj
Dr. Milan Randić (pogodbeno za 3 mesece / temporary for 3 months)

MLADI RAZISKOVALCI /
YOUNG RESEARCHERS
Špela Župerl

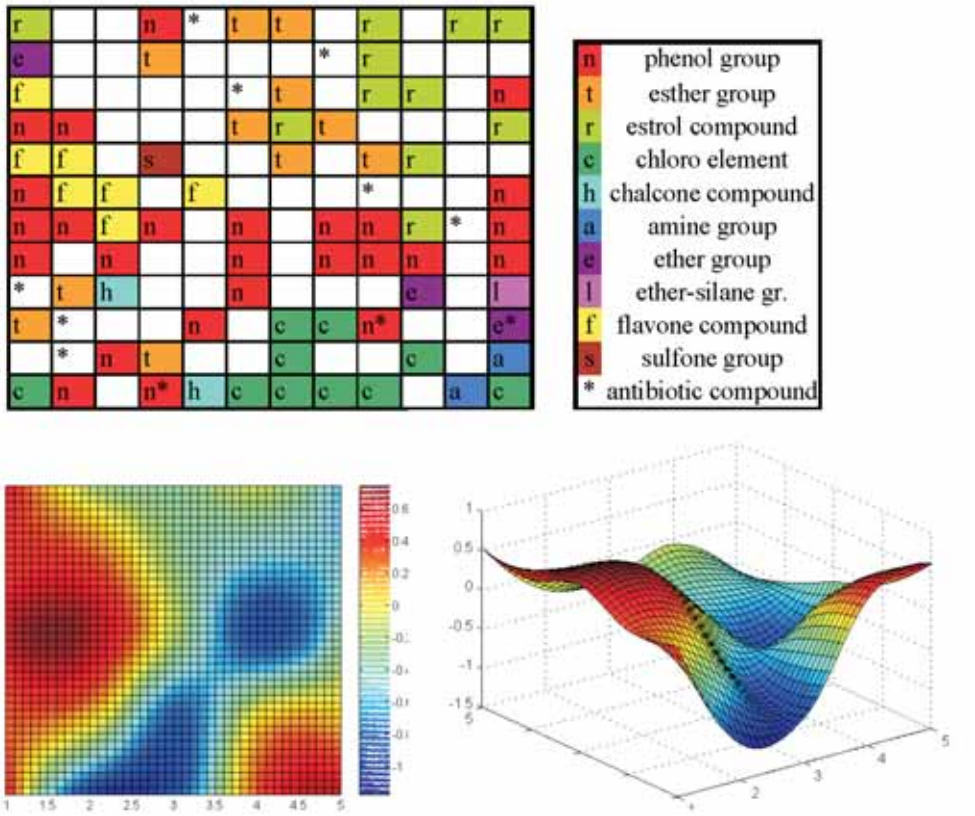
RAZISKOVALCI NA DO-DOKTORSKEM DELU IZ TUJINE /
YOUNG SCIENTISTS FROM ABROAD
Vinko Bandelj (1 mesec / 1 month)
Elisa Maran (3 mesece / 3 months)
Elena Boriani (6 mesecev / 6 months)
Morena Spreafico (4 mesece / 4 months)

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 nevronskih mrež v kemiji; študij strategij učenja nevronskih

RESEARCH ACTIVITIES

- Introduction of chemometrics, i.e., mathematical, statistical and computational methods for solving chemical problems, into the applicative, research, and control laboratories
- Modelling of chemical properties and processes in the field of QSAR and of data acquired from the hyphenated analytical techniques



SLIKA
Zgoraj: dvodimenzionalna mapa protitočne nevronske mreže dimenzije 12×12, v kateri so spojine iz učnega niza označene s simbolom skupine spojin oziroma funkcionalne skupine v kemijski strukturi (legenda desno), testirani antibiotiki pa so označeni z zvezdico.
Spodaj: Ravnina odgovorov, iz katere model poišče lastnost spojine, ki jo napoveduje. Vrednosti RBA se povečujejo od modre barve proti rdeči.

FIGURE
Upper part: 2-D map of counterpropagation neural network of dimension 12×12, with compounds labelled by their functional groups, while the tested antibiotics are labeled by an asterisk (see legend on the right).
Lower part: The response surface in which the predictions of the model are stored. The RBA values increase from blue towards the red color.

mrež in razvijanje ustreznih računalniških programov
- Raziskave na področju matematične kemije: uporaba diskretne matematike v strukturni kemiji
- Študij algoritmov in razvoj programskih paketov
- Uporaba kemometričnih metod v analizni kemiji: zagotavljanje in kontrola kvalitete (QA/QC)
- Raziskave 3D reprezentacij kemijske strukture za uporabo v QSAR
- Izobraževanje na področju kemometrije: v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani na dodiplomskem in podiplomskem nivoju
- Izobraževanje v okviru posebnih tečajev in šol v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Mariboru

BIBLIOGRAFIJA

24 izvirnih znanstvenih člankov
1 pregledni znanstveni članek
2 strokovna članka
1 poljudni članek
1 samostojni znanstveni sestavek v monografiji
4 objavljeni znanstveni prispevki na konferencah
11 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 prispevek na konferenci brez natisa
1 doktorat
4 uredništva revij

GLAVNI DOSEŽKI V LETU 2004

V letu 2004 smo začeli delo na programu Modeliranje relacij med kemijsko strukturo in lastnostjo snovi - QSAR – QSPR, ki je nastal z združitvijo dveh programov iz prejšnjih let, Modeliranje kemijskih lastnosti in procesov in Kemometrija. Za razširitev področja raziskav na programu smo dodali še nove usmeritve (kemijska sinteza, analitika in meroslovje). V

- Application of artificial neural network methods in chemistry, study of various ANN learning techniques and development of corresponding computer software
- Research in the field of mathematical chemistry: the application of discrete mathematics in structural chemistry
- Study of various algorithms and development of computer software
- Application of chemometric methods in analytical chemistry for quality control and quality assurance (QA/QC)
- Research of 3D structure representations for QSAR
- Education in chemometrics in collaboration with the Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia, on the pre and postgraduate levels
- Education in the form of special courses in the collaboration with the Faculty of Chemistry and Chemical Technology, University of Maribor, Slovenia

BIBLIOGRAPY

24 Original Scientific Articles
1 Review Article
2 Professional Articles
1 Popular Article
1 Scientific Article in a Monograph
4 Published Scientific Conference Contributions
11 Published Scientific Conference Contribution Abstracts
1 Unpublished Conference Contribution
1 Doctoral Dissertation
4 Editorships

IMPORTANT ACHIEVEMENTS IN 2004

In 2004 we started the work on the research program "Modelling of structure–property relationships – QSAR–QSPR", which is a complex interdisciplinary program established by joining two programs from previous years, Modelling of chemical properties and processes and

projektu sodelujejo Zavod za zdravstveno varstvo Maribor, Laboratorij za organsko sintezo in kemijo zdravil L08 na KI in nekaj zunanjih sodelavcev.

Raziskovalno delo Laboratorija za kemometrijo za leto 2004 je prikazano v 24 člankih in celi vrsti drugih publikacij. Med temi članki je tudi pomemben pregledni znanstveni članek s področja QSAR, Optimization algorithms and natural computing in drug discovery, Drug discovery today, Technologies, 2004, vol. 1, no. 3 (Lead optimization), ki podaja pregled metod optimizacije v načrtovanju zdravil. Napisan je bil na povabilo editorja revije.

Iz priložene bibliografije je razvidno, da smo bili, poleg raziskav na področju kemometrijskih metod in aplikacij, QSAR študij in obdelovanja velike količine podatkov okoljskih raziskav, dejavni tudi na področju teorije grafov z uporabo v strukturnih reprezentacijah, v proteomiki in genomiki. Razvoj indeksa podobnosti je omenjen v nadaljevanju kot pomemben dosežek laboratorija. Ravno tako smo uspešno vpeljali novo enolično grafično reprezentacijo proteinskih sekvenc na osnovi kodiranja nukleotidnih tripletov.

Med enega pomembnejših dosežkov v letu 2004 štejemo razvoj in objavo indeksa podobnosti med dvema proteomskima mapama. Študij podobnosti proteomskih map je pomemben zaradi analize rezultatov dvodimenzionalne elektroforeze, ki postaja pomemben pripomoček za študij proteinske situacije v celici (proteomika). Rezultat takšne meritve je dvodimenzionalna slika točk – proteomska slika, kjer vsaka točka predstavlja določen protein. Proteinska situacija se v celicah, ki so izpostavljene določeni kemikaliji, spremeni in to spremembo lahko zaznamo kot spremembo proteomske slike. Z uvedbo numeričnih indeksov (podobnostni indeks, Randićevi indeksi) smo opisali te spremembe na kvantitativen način.V literaturi smo našli podatke o proteomskih slikah mišjih jetrnih celic, ki so bila izpstavljena različnim koncentracijam peroksisomskega proliferatorja LY171883. Potek

"Chemometrics", enriched by the additional research areas (chemical synthesis, analytical chemistry with spectroscopy, and metrology). Into the joint program new directions were introduced through new links with other laboratories (Institute of Public Health Maribor, Slovenia, Laboratory for Medicinal Chemistry from National Institute of Chemistry, and some external collaborators).

The research in 2004 is presented in 24 papers and several other publications. Among papers we would like to stress the importance of a review article of J. Zupan et al.: Optimization algorithms and natural computing in drug discovery, Drug discovery today, Technologies, 2004, vol. 1, no. 3 (Lead optimization). It gives an overview of the optimization methods in drug design. It was written on an invitation of the editor of the journal.

It is evident from the bibliography of the group for 2004, that we were active in QSAR and chemometrics methods development and applications, in extracting information from large quantity of environmental data, as well as in the graph - theoretical research in the field of chemical structure representation, genomics and proteomics. The development of the similarity index in proteomics is mentioned below as one of the most important achievements in our laboratory. We also developed and introduced a unique graphical representation of protein based on nucleotide triplet codons.

One of the most important achievements in 2004 is the developments and publication of the similarity index between two proteomics maps. The study of similarity of proteomics maps is important because of the information extraction and analysis of 2D maps of proteins obtained by 2D electrophoresis, which is an important tool in the investigation of the proteins abundance in cells (proteomics). From 2D electrophoresis we obtain a map of points - proteomics image, in which each point represents an individual protein. The abundance of proteins in cells changes if treated by certain chemicals, which can be detected as a change

podobnostnega indeksa pri različnih koncentracijah kaže ramensko obliko, kar pomeni, da je efekt pri nižjih koncentracijah večji kot pri višjih. Pri tem bi lahko govorili o bifaznem odgovoru celic oziroma o hormeziji. Podoben odgovor ("oblika črke U") pri nizkih koncentracijah smo našli, ko smo proteomske slike opisanega sistema študirali z numeričnimi invariantami, osnovanimi na teoriji grafov.

V letu 2004 smo uspeli pridobiti soglasje vlade, da postanemo solastniki mednarodnega podjetja VICIM BV s sedežem na Nizozemskem. Podjetje je bilo ustanovljeno v nadaljevanju Evropskega projekta VICIM iz evropskega 5. okvirnega programa, katerega partner je bila tudi naša skupina za kemometrijo. Podjetje bo opravljalo kemometrijske in metrološke usluge za naročnike tudi po izteku projekta.

V letu 2004 smo se uspeli vključiti v dva nova evropska projekta, in sicer TRACE (FP6-2003-FOOD-2-A) in IBAAC (MCRTN –CT-2003-505020).

Pod mentorstvom naših sodelavcev in v sodelovanju s Fakulteto za kemijo in kemijsko tehnologijo Univerze v Ljubljani je bila v letu 2004 končana doktorska disertacija Marjana Tušarja, Izboljšave pri modeliranjih kemijskih problemov z nevronskimi mrežami.

RAZVOJ *in silico* MODELA ZA OCENO ŠKODLJIVOSTI KEMIKALIJ

Kot ilustracijo bomo predstavili le eno od značilnih QSAR raziskav, izvršenih leta 2004. To delo (E. Maran, M. Novič, P. Barbieri, J. Zupan, Application of counter-propagation artificial neural network for modelling properties of fish antibiotics. SAR QSAR environ. res., 2004, vol. 15, no. 5/6, str. 469-480) je zanimivo s stališča uvajanja *in silico* metod za ocenjevanje kemikalij. Ocena tveganja zaradi toksičnosti posameznih spojin je pomemben podatek za proizvajalce kemikalij, za njihove uporabnike oziroma v splošnem za okolje, in zato tudi za evropsko zakonodajo. Število in poraba kemikalij v svetu strmo

of the proteomics image. The introduction of numerical indices (similarity index, Randić index) offers a quantitative measure for the description of the changes. From the literature we collected the proteomics maps recorded from mice liver cells. The liver cells have been disposed to different concentrations of peroxisome proliferators LY171883. The behaviour of our similarity index shows a shoulder shape, what means that the effect at very low concentrations is larger than at higher concentrations. The effect could be explained by the hormesis - a well known dose response phenomenon characterized by a low dose stimulation, high dose inhibition. The same behaviour is found also with different graph - theoretical invarians obtained from proteomics maps.

In 2004 we succeeded to obtain the government agreement to become a shareholder of VICIM BV, with a headquater in the Netherland. The company VICIM BV was established as a continuation of the EU project in the 5th framework, in which our group participated as one of the partners. The company is designed for consulting and helping industry with chemometric and metrological expertise after the outgoing project VICIM.

In 2004 we succeeded to join two new European projects, TRACE (FP6-2003-FOOD-2-A) and IBAAC (MCRTN –CT-2003-505020).

DEVELOPMENT OF *in silico* MODEL FOR ASSESSMENT OF CHEMICALS

For illustration we will present one of typical QSAR research completed in 2004. This work (E. Maran, M. Novič, P. Barbieri, J. Zupan, Application of counter-propagation artificial neural network for modelling properties of fish antibiotics. SAR QSAR environ. res., 2004, vol. 15, no. 5/6, pg. 469-480) is interesting from a viewpoint of introducing *in silico* methods for assessment of chemicals. Risk assessment due to toxic effects of chemicals is important information for the producers, customers, and environment; consequently it is important for the European legislation. Number and consump-

narašča, zato bi dolgotrajne in drage ter etično sporne *in vivo* teste želeli nadomestiti z računskimi metodami ocene toksičnih lastnosti kemikalij. V zgoraj omenjeni raziskavi smo izbrali niz 132 spojin, motilcev žlez z notranjim izločanjem s poznano afiniteto (RBA) do estrogen receptorja. Za vsako spojino smo izračunali 281 strukturnih deskriptorjev (konstitucijskih, topoloških, geometrijskih, kvantno kemijskih ter porazdelitveni koeficient med vodo in oktanolom) in s pomočjo protitočne nevronske mreže zgradili model za napovedovanje RBA za strukturno sorodne spojine. Model je bil ocenjen z navzkrižnim testom na 132 spojinah podatkovnega niza. Korelacijski koeficient med izmerjenimi in z modelom napovedanimi vrednostmi je r = 0.99, pri navzkrižnem testu z izpuščanjem po eno spojino v vsakem od 132 ciklov pa dobimo vrednost r_{cv} = 0.91.

Značilnost modelov na osnovi protitočnih nevronskih mrež je v tem, da se spojine najprej organizirajo v dvodimenzionalnih mapah glede na podobnost kemijske strukture. Merilo podobnosti je Evklidska razdalja med vektorji strukturnih deskriptorjev posameznih molekul. S pomočjo zgrajenega modela smo preizkusili 15 spojin, ki jih uporabljajo kot antibiotike v ribjih farmah, kako močno bi se vezale na estrogenski receptor (Slika). Za vsako od 15 spojin smo morali izračunati 281 strukturnih deskriptorjev na enak način kot za podatkovni niz 132 spojin. 15 testnih spojin smo testirali z našim modelom in dobili napovedane vrednosti RBA ter razdaljo med spojino (281 dimenzionalni vektor deskriptorjev) in enako dimenzionalnim nevronom. S pomočjo tega nevrona namreč zgrajeni model napove željeno lastnost spojine. Iz razdalje smo izračunali faktor zanesljivosti za napoved vsake od 15 testiranih spojin. Večja ko je razdalja, manjša je zanesljivost napovedi. Z drugimi besedami to pomeni, da je napoved spojine, pri kateri smo dobili veliko razdaljo, nezanesljiva, ker naš model ni bil zgrajen s strukturno dovolj podobnimi spojinami.

tion of chemicals increases rapidly, so it would be favourable to diminish expensive and ethically questionable *in vivo* tests and substitute them in a large part by computational methods. We have chosen in the study mentioned above a set of 132 chemicals, endocrine disrupting chemicals with known binding affinity (RBA) to estrogen receptor. 281 structural descriptors (constitutional, topological, geometrical and quantum chemical and log P) were calculated for each compound and a model based on counterpropagation neural network was constructed. The model was tested by a cross - validation test on all 132 compounds. The correlation coefficients of the training data and of the cross - validation procedure were 0.99 and 0.91, respectively.

The counerpropagation neural networks are trained in such a way, that in the first step the compounds are organised in a 2D map regarding the similarity between the structures. The similarity measure is the Euclidean distance between the vectors containing structural descriptors. With the constructed model 15 compounds used as fish antibiotics were tested for their affinity to estrogen receptor (Figure). First we had to calculate 281 descriptors for all 15 molecules on the same way as for the original dataset. From our model we obtained the predicted RBA values of 15 antibiotic molecules and a distance between the 281- dimensional structural representation of each molecule and the same dimensional neuron, which was excited by the tested molecule and defines the predicted value. The obtained distance was a basis for the calculation of the reliability factor of individual predictions. The grater the distance, the lower is the reliability coefficient. In other words, if we obtain a large distance for prediction of a certain molecule, this prediction is unreliable because the model was not trained with the compounds similar to the one tested.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Lek d.d., Ljubljana

Potencialni industrijski uporabniki so 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

v mednarodnih projektih:

- Projekt IMAGETOX (Intelligent Modelling Algorithms for General Evaluation of TOXicities) za 5. okvirni projekt EU; zaključen v začetku leta
- Marie Curie Host Fellowships - Training Site, za 3 študente po eno štipendijo na leto (Contract No HPMT-CT-2001-00240)
- Projekt VICIM (Virtual Institute of Chemometrics and Industrial Metrology, Contract No.: G7RT-CT-2001-05067); v zaključni fazi
- Projekt TRACE (FP6-2003-FOOD-2-A) (Tracing Food Commodities in Europe); začetna faza
- Projekt IBAAC (MCRTN –CT-2003-505020) (An Integrated Biomimetic Approach to Asymmetric Catalysis); začetek sredi leta
- Bilateralni projekt v okviru programa znanstvenega in tehnološkega sodelovanja med vlado Republike Slovenije in vlado Italijanske Republike za obdobje 2002 do 2005 z naslovom "QSAR študije na PCB in PAH spojinah za oceno tveganja v obmorskih mestnih območjih"; nosilca: dr. Marjan Vračko in dr. Pierluigi Barbieri
- Bilateralni projekt v okviru slovensko - indijskega programa znanstveno tehnološkega sodelovanja 2004 - 2005 z naslovom "QSAR protituberkuloznih spojin: primerjave statističnih modelov in nevronskih mrež";

INTERNATIONAL COLLABORATION

- Project IMAGETOX (Intelligent Modelling Algorithms for General Evaluation of TOXicities) in 5. EU framework; closed in 2004
- Marie Curie Host Fellowships - Training Site, for 3 years, 1 student each year (Contract No. HPMT-CT-2001-00240)
- Project VICIM (Virtual Institute of Chemometrics and Industrial Metrology (Contract No. G7RT-CT-2001-05067); in closing phase
- Project TRACE (FP6-2003-FOOD-2-A) (Tracing Food Commodities in Europe); starting phase
- Projekt IBAAC (MCRTN –CT-2003-505020) (An Integrated Biomimetic Approach to Asymmetric Catalysis); started during the year
- Bilateral projects in the frame of Scientific and technological cooperation between Slovenia and Italy for the period 2002 - 2005 entitled "QSAR studies on PCB and PAH compounds for risk assessment in costal urbal regions"; principal investigators: Dr. Marjan Vračko and Dr. Pierluigi Barbieri
- Bilateral projects in the frame of Slovenian - Indian intergovernmental science and technology cooperation programme for the period 2004 - 2005 entitled "QSAR of antituberculosis drugs: A comparison of statistical and neural nets models"; principal investigators: Dr. Marjan Vračko and Dr. Manish Bagshi
- Bilateral projects in the frame of Scientific and technological cooperation between Slovenia and Macedonia for the period 2004 - 2006 entitled "Quantitative Structure-Activity Relationship Studies of HIV-1 Inhibitor Molecules"; principal investigators Dr. Marjana Novič and Dr. Igor Kuzmanovski

IMPORTANT INSTRUMENTS

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

nosilca: dr. Marjan Vračko in dr. Manish Bagshi

- Bilateralni projekt v okviru znanstveno - tehnološkega sodelovanja med Republiko Slovenijo in Republiko Makedonijo v letih 2004, 2005 in 2006 z naslovom "Študij relacij med kemijsko strukturo in aktivnostjo molekul, ki inhibirajo HIV-1"; nosilca: dr. Marjana Novič in dr. Igor Kuzmanovski

POMEMBNI INŠTRUMENTI IN OPREMA

- Računalniška učilnica s 30 sedeži in 16 osebnimi računalniki
- DIONEX-DX500 ionski kromatograf

L04

Laboratorij za analizno kemijo

Laboratory for Analytical Chemistry

VODJA / HEAD
Dr. Božidar Ogorevc

RAZISKOVALCI / RESEARCHERS
Doc. dr. Mirko Bizjak (do februarja / until february)
Dr. Bojan Budič
Dr. Johannes T. van Elteren
Dr. Irena Grgić
Dr. Samo Hočevar
Dr. Miroslav Kovačevič (od marca / since march)
Doc. dr. Milko Novič
Dr. Janja Turšič

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Mag. Boštjan Podkrajšek
Marija Slavec (od decembra / since december)

TEHNIČNO OSEBJE / TECHNICAL STAFF
Nuša Verbič
Breda Novak
Lidija Živec (polovični čas / part time)
Olga Gorše (polovični čas - do septembra / part time - until september)
Vesna Lenarčič (polovični čas - od oktobra / part time - since october)

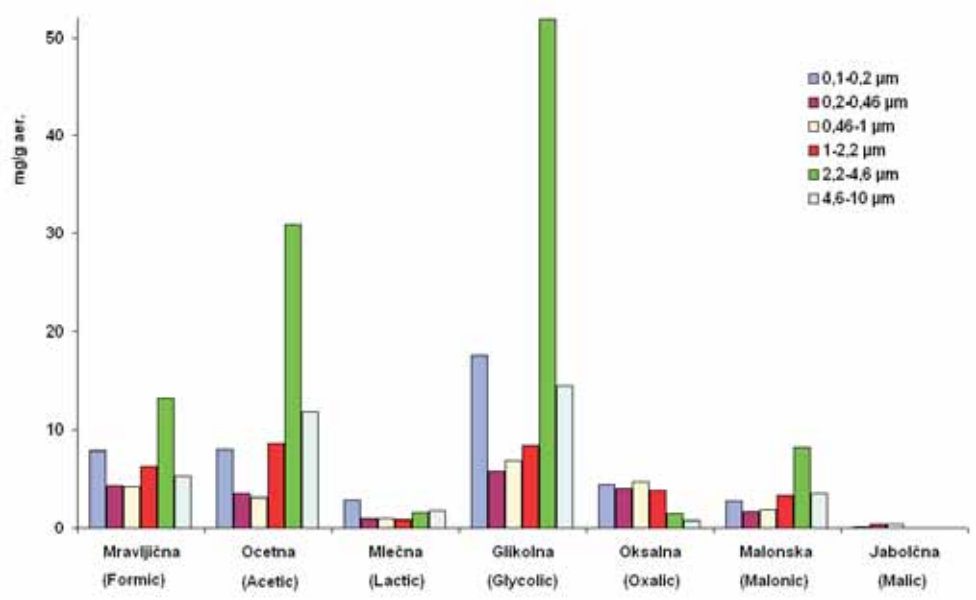
PODOKTORSKI GOSTJE / POSTDOCTORAL FELLOWS
Dr. Emily A. Hutton (Irska / Ireland)

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 zvrsti 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 v povezavi z ICP-masno spektroskopijo), ionska kromatografija, kemijski procesi v atmosferski vodni fazi, vzorčevanje in karakterizacija atmosferskih aerosolov (po velikostnih frakcijah), ICP-atomska emisijska spektrometrija, priprava vzorcev (razklop v MW-peči in sekvenčna / selektivna

RESEARCH ACTIVITIES

The Laboratory for Analytical Chemistry'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 Laboratory team is very broad and covers amongst others electrochemistry (micro-electrodes and sensors), hyphenated techniques (such as liquid chromatography with ICP-mass spectroscopy), ion chromatography, chemical processes in atmospheric aqueous phase, sampling and characterization of size-segregated atmospheic aerosols, ICP-atomic emission spectrometry, sample preparation (MW-assisted digestion and sequential/



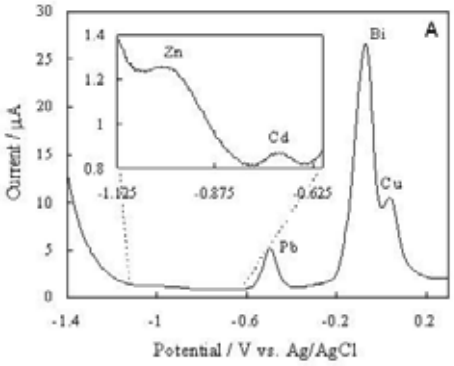
SLIKA 1
Povprečne koncentracije vodotopnih karboksilnih kislin (mg g-1aerosola) v aerosolnih delcih po velikostnih razredih zbranih med merilno kampanjo v Ljubljani 2004. Karboksilne kisline imajo zaviralni učinek na oksidacijo SO_2 v atmosferski vodni fazi, kar lahko omogoča transport nezreagiranega SO_2 na daljše razdalje.

FIGURE 1
Average concentrations of water soluble carboxylic acids (mg g-1aerosol) in size segregated aerosol particles collected during the campaign in Ljubljana 2004. Carboxylic acids inhibit SO_2 oxidation in atmospheric waters, which can lead to a longer-range transport of un-reacted SO_2.

ekstrakcija) in modeliranje (ekstrakcijskih in separacijskih procesov).
Dejavnost Laboratorija zajema tudi pogodbeno delo in storitve za neposredne industrijske in druge partnerje, kar vključuje razvoj in izboljšave metod ter analize vseh vrst vzorcev (okoljski, industrijski, biološki) in določevanje praktično vseh elementov periodnega sistema kot tudi mnogih anorganskih in organskih ionov.
Več informacij na spletni strani: http://www.ki.si/lab/l04/

BIBLIOGRAFIJA

15 izvirnih znanstvenih člankov
7 objavljenih znanstvenih prispevkov na konferencah
17 objavljenih povzetkov znanstvenih prispevkov na konferencah
3 končna poročila o rezultatih raziskav



SLIKA 2

Validacija bizmutove tankoslojne elektrode (BiFE) za direktno določevanje ultrasledov kadmija v ekstraktih vzorcev tal z uporabo masne spektrometrije z induktivno sklopljeno plazmo (ICP-MS). (A) Tipični anodni stripping voltamogram (ASV), posnet z in situ priporavljeno BiFE na primeru vzorca tal ekstrahiranega z 0.1 M HNO_3 , po razredčitvi (1+3) z 0.1 M acetatnim pufrom (pH 4.5). (B) Primerjava rezultatov ASV (z BiFE) in ICP-MS meritev kadmija v ekstraktu vzorca tal po ekstrakciji z 0.1 M HNO_3 pri različnih razmerjih volumna in mase (A-E: 10-50 ml/g). Pomen BiFE je v možnosti njene uporabe v meritvah na terenu in v uporabi ASV kot alternativne metode.

selective extraction), and modelling (extraction and separation processes).
Laboratory activities also encompass contract work and special analytical services for industrial and other partners including development and adaptation of methods and analysis of all kinds of samples (environmental, industrial, biological) and determination of practically all elements of the periodic table as well as many inorganic and organic ions.
More information is available at: http://www.ki.si/lab/l04/

BIBLIOGRAPHY

15 Original Scientific Articles
7 Published Scientific Conference Contributions
17 Published Scientific Conference Contribution Abstracts

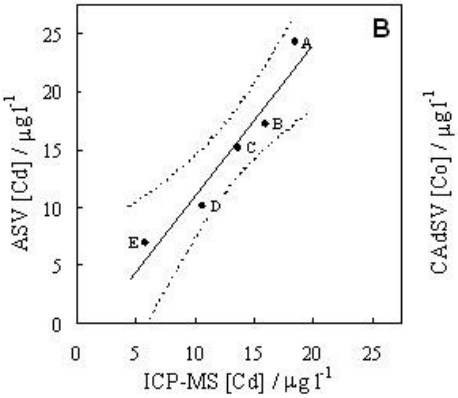


FIGURE 2

Validation of bismuth film electrode (BiFE) for direct determination of ultratrace levels of cadmium in soil extracts using inductively coupled plasma - mass spectrometry (ICP-MS). (A) Typical anodic stripping voltammogram (ASV) obtained at the in situ prepared BiFE for a soil extracted with 0.1 M HNO_3 and diluted (1+3) with 0.1 M acetate buffer (pH 4.5). (B) Comparison of results obtained with ASV (at the BiFE) and ICP-MS for cadmium in soil extracted with 0.1 M HNO_3 at different volume to mass ratios (A-E: 10-50 ml/g). The significance of BiFE is the possibility of its use in decentralized/on-field measurements and in the use of ASV as an alternative method.

4 elaborati, predštudiji, študiji
2 doktorata

Raziskovalci Laboratorija za analizno kemijo so v letu 2004 sodelovali na eni domači konferenci (Kemijski dnevi v Mariboru) s 3 prispevki in na 9 mednarodnih znanstvenih konferencah z 20 prispevki.

GLAVNI DOSEŽKI V LETU 2004

- Razvili smo nov način direktnega uvajanja organskih topil v razpršilno komoro elementnega masnega spektrometra (ICP-MS), s čimer povečamo delež ionizacije elementov z visokim ionizacijskim potencialom (Se, P in As). S tem smo povečali občutljivost in znižali meje detekcije za te elemente.
- Vpeljali in validirali smo EPA 321.8 metodo za določevanje vsebnosti bromata v pitni vodi, ki temelji na sklopljenem sistemu ionska kromatografija - elementna masna spektrometrija (IC-ICP-MS).
- Dokazali smo, da lahko z dodajanjem spojin, ki vsebujejo ogljik močno povečamo občutljivost detekcije fosforja z ICP-MS. V sodelovanju z Inštitutom Rudjer Bošković , Zagreb, Hrvaška smo identificirali poliatomske ione, ki motijo meritve pri atomski masi fosforja. Na podlagi teh raziskav smo za industrjskega partnerja razvili IC-ICP-MS metodo za določevanje fosfonatov v vodikovem peroksidu.
- Realne aerosole, ki smo jih poprej vzorčili v obmorskem in urbanem okolju, smo v posebni reakcijski komori izpostavili mešanici SO_2/zrak ali SO_2/NH_3/zrak pri različnih relativnih vlagah in ugotovili pomembno dejstvo, da je njihova reaktivnost odvisna od velikosti delcev in s tem povezane sestave.
- V sodelovanju z ameriškim partnerjem smo razvili elektrokemijski senzor za detekcijo ultra-sledov 2,4,6-trinitrotoluena (TNT) na osnovi elektrode, modificirane z ogljikovimi nanocevkami, ki omogoča merjenje izredno nizkih koncentracij TNT v morski vodi.

3 Final Research Reports
4 Treatises, Preliminary Studies, Studies
2 Doctoral Dissertations

IMPORTANT ACHIEVEMENTS IN 2004

- A new mode for the direct introduction of organic solvents into the spray chamber of ICP-MS system was developed. It is used for enhancement of the ionisation rate of elements with high ionisation potentials (Se, P and As) enabling higher sensitivity and lower detection limits for these elements.
- We introduced and validated the EPA 321.8 method, which is based on hyphenation of ion chromatography and element mass spectrometry (IC-ICP-MS), for the detection of low levels of bromate for its determination in drinking water.
- We proved that the addition of carbon containing compounds significantly improves the sensitivity of the ICP-MS detection of phosphorus. In collaboration with the Rudjer Bošković Institute (Zagreb, Croatia) we identified polyatomic ions, which interfere with measurements at the atomic mass of phosphorus. Based on these findings, we developed an IC-ICP-MS method for the determination of phosphonates in hydrogen peroxide for an industrial partner.
- Atmospheric aerosols, previously collected in marine and urban environments, were exposed in a special reaction chamber to SO_2/air or SO_2/NH_3/air gas mixtures at different relative humidities. We discovered an important fact, namely that the reactivity of aerosols significantly depends on the particle size, which is related to their chemical composition.
- In collaboration with our American partner we developed an electrochemical sensor for the detection of ultra-trace levels of 2,4,6 trinitrotoluene (TNT) based on a carbon nanotube-modified electrode, which allows detection of very low concentrations of TNT in sea water.

- Razvili smo elektrokemijski mikro-biosenzor za glukozo, ki temelji na elektrodi iz ogljikovega vlakna, ki je modificirana z manganovim dioksidom in encimom glukoza-oksidazo ter dodatno prekrita s polimerom nafionom. Ta mikro - biosenzor deluje v koncentracijskem območju, ki odgovarja realnim fiziološkim koncentracijam glukoze v človeškem organizmu.
- Prvi smo razvili trdo bizmutovo elektrodo, ki omogoča merjenje nekaterih težkih kovin v sledovih v primerih, ko je uporaba in situ ali ex situ pripravljene bizmutove tankoslojne elektrode nezaželjena ali celo nemogoča.
- Izvedli smo kritično evalvacijo metodologij za ekstrakcijo kovin iz vzorcev tal in ugotovili, da običajno uporabljeno razmerje mase vzorca in volumna ekstraktanta lahko privede tudi do 50% prenizkih izkoristkov ekstrakcije. Zato smo razvili nov teoretičen model osnovan na linearni adsorpcijski izotermi, ki daje točne rezultate glede maksimalnih možnih ekstrakcij kovin pri danih pogojih.
- Izdelali smo nov koncept možnosti ekstrakcije kemijsko razpoložljivih kovin in polkovin iz vzorcev tal, ki temelji na kombiniranju absolutnih pristopov z uporabo sledilcev (radioaktivnih ali stabilnih) in "približnih" pristopov z uporabo bolj običajnih ekstrakcijskih tehnik.
- S primerjavo stripping voltametrične in spektroskopske (ICP-MS) metode smo validirali in potrdili uporabnost bizmutove tankoslojne elektrode za direktne določitve kobalta in kadmija v μg/L koncentracijskem območju v ekstraktih vzorcev tal.
- Za določitev arzenovih spojin v vzorcih lišajev (Parmelia sulcata) smo uporabili sekvenčno ekstrakcijo v kombinaciji s tekočinsko kromatografijo sklopljeno z atomsko fluorescenčno spektrometrijo (HPLC-HGAFS) ter ugotovili, da anorganske spojine arzena močno prevladujejo, prisotnost manjših količin organskih arzenovih spojin pa kaže na možnost biotransformacije anorganskega arzena v lišajih.

- We developed an electrochemical glucose micro-biosensor based on a carbon fiber micro-electrode modified with manganese dioxide and the enzyme glucose-oxidase, and additionally coated with Nafion polymer. This micro-biosensor allows glucose measurement at concentrations typical for its physiological levels in human body.
- We first introduced the bismuth bulk electrode for the measurement of some trace heavy metals, particularly in those situations when the application of in situ or ex situ bismuth film electrodes is unfavorable or even impossible.
- We performed a critical assessment of solid-liquid extraction methodologies for the determination of metals in soil samples and found that the volume to mass ratios commonly used may lead to as much as 50% too low extraction yields. We therefore developed a theoretical framework based on linear adsoption isotherm behaviour to allow a correct maximal metal extractability from soil.
- We developed a new concept of retrieval of the chemically available metal(loid) concentration in soil based on combination of exact approaches using (radioactive or stable) tracers and "approximate" approaches using more conventional extraction techniques.
- By comparing stripping voltammetric and spectroscopic (ICP-MS) methods we validated and approved the suitability of the bismuth film electrode for the determination of cadmium and cobalt at μg/L levels in soil extracts.
- A sequential extraction in combination with liquid chromatography coupled with atomic fluorescence spectrometry (HPLC-HGAFS) was applied for the determination of arsenic species in lichen transplants and airborne particulate matter. Inorganic forms of arsenic were present in significant amounts in most of the samples while organic forms of arsenic were identified only in lichens, which may indicate biotransformation of inorganic arsenic.

- Določili smo inhibicijske parametre pri oksidaciji S(IV) katalizirani z Mn(II) v prisotnosti nizko molekularnih karboksilnih kislin, ki smo jih izbrali na osnovi analize realnih atmosferskih aerosolov po velikostnih frakcijah.
- Prvi smo razvili kinetski model, s katerim opišemo vpliv vseh preiskanih karboksilnih kislin na katalitsko oksidacijo S(IV) v celotnem preiskanem koncentracijskem območju pri pH 3,5 in 4,5.
- V sodelovanju z avstrijskim partnerjem smo izvedli dve merilni kampanji zbiranja atmosferskih aerosolov urbanega izvora (Dunaj, Ljubljana) z uporabo šeststopenjskega kaskadnega impaktorja (velikost delcev med 100 nm in 10 μm). Po natančni kemijski karakterizaciji bodo vzorci uporabljeni za študij reaktivnosti realnih aerosolov.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V letu 2004 smo sodelovali z vrsto industrijskih partnerjev v okviru večjih pogodb ali naročil za kemijsko (elementno) analizo različnih vzorcev iz proizvodnje ali okolja, ki zahtevajo posebno znanje in izkušnje ter specialno instrumentacijo. Med najpomembnejše industrijske partnerje tovrstnega sodelovanja v letu 2004 sodijo:

- Salonit Anhovo d.d., Deskle; Petrol d.d., Ljubljana; Pivovarna Union d.d., Ljubljana; Komplast d.o.o., Ljubljana; Melamin d.d., Kočevje; Eta d.o.o., Cerkno; Lek d.d., Ljubljana; Iskra EMS, Šentjernej; Belinka Perkemija d.o.o., Ljubljana; Helios d.o.o., Domžale; Interdent Celje; AET Tolmin; Nuklearna elektrarna Krško; Pikas Tolmin; Sava Trade d.d., Ljubljana idr.

Sodelovanje z neindustrijskimi partnerji v letu 2004 je zajemalo pogodbeno ali drugačno razvojno in raziskovalno delo z naslednjimi neposrednimi partnerji:

- Agencija Republike Slovenije za okolje, Ljubljana; Elektroinštitut Milan Vidmar, Ljubljana; Zavod za zdravstveno varstvo, Celje;

- We determined the inhibition parameters for the kinetics of S(IV) oxidation catalyzed by Mn(II) in the presence of low weight carboxylic acids, chosen on the basis of analysis of size-segregated atmospheric aerosols.
- We were the first to derive a kinetic model which predicts the influence of all investigated acids on catalyzed S(IV) oxidation over the entire examined concentration range at pH 3.5 and 4.5.
- In collaboration with our Austrian partner we collected size-segregated aerosol samples in urban areas (Vienna, Ljubljana) using six-stage cascade impactors (particle size 100nm-10μm). After chemical and physical characterisation, these aerosols will be used for reactivity studies.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

In 2004 we collaborated with numerous industrial partners in the frame of larger contracts and orders for chemical (elemental) analysis of various samples from industrial processes and the environment, which require the analytical expertise and special instrumentation that the Laboratory for Analytical Chemistry can provide owing to its research activity. A list of the most important industrial partners in 2004 comprises:

- Salonit Anhovo d.d., Deskle, Slovenia; Petrol d.d., Ljubljana, Slovenia; Pivovarna Union d.d., Ljubljana, Slovenia; Komplast d.o.o., Ljubljana, Slovenia; Melamin d.d., Kočevje, Slovenia; Eta d.o.o., Cerkno, Slovenia; Lek d.d., Ljubljana, Slovenia; Iskra EMS, Šentjernej, Slovenia; Belinka Perkemija d.o.o., Ljubljana, Slovenia; Helios d.o.o., Domžale, Slovenia; Interdent Celje, Slovenia; AET Tolmin, Slovenia; Nuklear Power Plant Krško, Slovenia; Pikas Tolmin, Slovenia; Sava Trade d.d., Ljubljana, Slovenia etc.

Collaboration with non-industrial partners in 2004 represented contract and other development and research work with the following partners:

Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani; Enota za patologijo prehrane in higieno okolja (NVI, Veterinarska fakulteta Univerze v Ljubljani); Inštitut Jožef Stefan, Ljubljana; Zavod za gradbeništvo Slovenije, Ljubljana; Laboratorij za astrofiziko osnovnih delcev in Laboratorij za raziskave v okolju (Politehnika, Nova Gorica); Očesna klinika (Medicinska fakulteta Univerze v Ljubljani); Laboratorij za raziskavo možganov (Inštitut za patološko fiziologijo, Medicinska fakulteta Univerze v Ljubljani) idr.

V letu 2004 smo pridobili in pričeli izvajati raziskovalno - aplikativni projekt z naslovom "Vpliv emisijskih virov na onesnaženje zraka s trdnimi delci". Trajanje: 2004 - 2007. Sodelovanje med Kemijskim inštitutom, Elektroinštitutom Milan Vidmar, Ljubljana in Termoelektrarno Šoštanj. Nosilka projekta: I. Grgić.

MEDNARODNO SODELOVANJE

V letu 2004 so bili sodelavci Laboratorija za analizno kemijo vključeni v naslednje mednarodne projekte:

- INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change"); program evropske znanstvene fondacije 2004 - 2008; nacionalna koordinatorka in članica vodstvenega odbora: I. Grgić
- Raziskovalni projekt financiran s strani EC 6FP, Sekcija "Support for research Infractures -Integrated Infrastructure Initiative" z naslovom "Integration of European Simulation Chambers for Investigating Atmospheric Processes" (EUROCHAMP), vključeni kot "associate users"
- COST Action 633 »Particulate Matter: Properties Related to Health Effects«, projekt poteka v okviru Evropske znanstvene fondacije; trajanje: 2002 - 2007; nacionalna koordinatorka ter podpredsednica COST 633: J. Turšič
- Bilateralni projekt z naslovom "Heterogene reakcije atmosferskih aerosolov pri kontro-
- Agency of the Republic of Slovenia for the Environment, Ljubljana, Slovenia; The Milan Vidmar Electroinstitute, Ljubljana, Slovenia; Public Health Institute, Celje, Slovenia; Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia; Unit for Pathology of Animal Nutrition and Environmental Hygiene (NVI, Veterinary Faculty, University of Ljubljana, Slovenia); Jozef Stefan Inštitute, Ljubljana, Slovenia; Slovenian National Building and Civil Engineering Institute, Ljubljana, Slovenia; Laboratory for Astroparticle Physics and Laboratory for Environmental Research (Nova Gorica Polytechnic Slovenia); Eye Clinic (Medical School, University of Ljubljana, Slovenia); Laboratory for Brain Research (Institute of Pathophysiology, Medical School, University of Ljubljana, Slovenia) etc.

In 2004 we started an applied research project entitled "Influence of emission on ambient air pollution by particulate matter"; duration: 2004 - 2007. A collaborative research between National Institute of Chemistry, The Milan Vidmar Electroinstitute, Ljubljana, Slovenia and the Thermo-power plant Šoštanj, Slovenia. Principal Investigator: I. Grgić.

INTERNATIONAL COLLABORATION

In 2004 the Laboratory for Analytical Chemistry team members were involved in the following international research projects:

- An European Science Foundation Program INTROP ("Interdisciplinary Tropospheric Research: from the Laboratory to Global Change"); duration: 2004 - 2008; national coordinator and member of the Steering Committee: I. Grgić
- Research project funded within the EC 6FP, Section Support for Research Infractures -Integrated Infrastructure Initiative: "Integration of European Simulation Chambers for Investigating Atmospheric Processes" (EUROCHAMP), involved as associate users

liranih eksperimentalnih pogojih značilnih za meglico - drugi del" v okviru slovensko - avstrijskega znanstvenega sodelovanja 2004 - 2005; partner: prof. R. Hitzenberger, Inštitut za eksperimentalno fiziko, Univerza na Dunaju, Avstrija; nosilka projekta: I. Grgić

- Bilateralni projekt z naslovom "Novi materiali za elektrokemijsko detekcijo v stripping analizi" v okviru slovensko - češkega znanstvenega sodelovanja 2004 – 2005; partner: prof. K. Vytras, University of Pardubice, Pardubice, Češka; nosilec projekta: B. Ogorevc
- Bilateralni projekt z naslovom "Študij sestave, strukture in uporabnosti naravnih zeolitov v sistemih za zaščito okolja" v okviru slovensko - hrvaškega znanstvenega sodelovanja 2003 – 2004; partner: prof. Š. Cerjan - Štefanović, Vseučilišče iz Zagreba, Hrvaška; nosilec projekta: Mi. Novič
- dr. N. Avdalović, Dionex Corporation, CA, ZDA; nosilec projekta: Mi. Novič
- Bilateralni projekt z naslovom "In situ monitoring approaches for soils contaminated with arsenic and other toxic elements" (PSP-22/2004) v okviru slovensko - britanskega znanstvenega sodelovanja 2004; partner: prof. H. J. Glass, University of Exeter, Velika Britanija

POMEMBNI INŠTRUMENTI IN OPREMA

- Masni spektrometer z induktivno sklopljeno plazmo (ICP-MS, Hewlett Packard, model HP 4500 PLUS) s HPLC modulom in UV/Vis spektrometrom (DAD, Agilent, 1100 Series)
- Atomski emisijski spektrometer z induktivno sklopljeno plazmo (ICP-AES, Thermo Jarrell Ash, Model Atomscan 25) opremljen z ultrazvočnim razpršilcem (Cetac, model U-6000 AT)
- Dva sistema za ionsko kromatografijo (IC) s konduktometrično in spektrofotometrično detekcijo
- Pretočno injekcijski analizator (ASIA Ismatec)
- Več modularnih računalniško vodenih

- 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
- Bilateral project entitled "Heterogeneous Reactions of Atmospheric Aerosols under Controlled Experimental Conditions Typical for Haze - Part 2" in the frame of S&T cooperation between Slovenia and Austria 2004 - 2005; partner: Prof. R. Hitzenberger, Institut for Experimental Physics, University of Vienna, Austria; p.i.: I. Grgić
- Bilateral project entitled "New Materials for Electrochemical Detection in Stripping Analysis" in the frame of S&T cooperation between Slovenia and Czeck Republic 2004 - 2005; partner: Prof. K. Vytras, University of Pardubice, Pardubice, Czech Republic; p.i.: B. Ogorevc
- Bilateral project entitled "Study of Composition, Structure and Application of Natural Zeolites in Environment Protection Systems" in the frame of S&T cooperation between Slovenia and Croatia 2003 - 2004; partner: Prof. Š. Cerjan-Štefanović, Faculty of Chemical Engineering and Technology, University of Zagreb, Croatia; p.i.: Mi. Novič
- Bilateral project entitled "Modeling of Separation Mechanisms in Modern Ion Chromatography" in the frame of S&T cooperation between Slovenia and USA 2003 - 2004; partner: Dr. N. Avdalović, Dionex Corporation, CA, USA; p.i.: Mi. Novič
- Bilateral project entitled "In situ monitoring approaches for soils contaminated with arsenic and other toxic elements" (PSP-22/2004) in the frame of S&T cooperation between Slovenia and UK 2004; partner: Prof. H. J. Glass (University of Exeter in Cornwall, UK)

MAJOR EQUIPMENT

- Inductively coupled plasma mass spectrometer (ICP-MS, Hewlett Packard, Model HP

elektrokemijskih sistemov (Autolab, Eco Chemie)
- Invertni optični mikroskop (Eclipse, Nikon)
- Orodja za izdelavo mikroelektrod (aparat za vlečenje kapilar, mikromanipulator idr.)
- Reakcijska komora za raziskovanje reaktivnosti aerosolskih delcev pod kontroliranimi pogoji
- Oprema za vzorčevanje aerosolov z Bernerjevimi nizkotlačnimi kaskadnimi impaktorji
- CHN/S elementni analizator (CE 440, Leeman Labs Inc.)
- Mikrovalovna peč za razklope (MLS 1200 MEGA, Milestone)

IZOBRAŽEVANJE
- Doktorat: mag. M. Kovačevič, univ. dipl. kem.; naslov disertacije: "Uporaba sklopljenega sistema tekočinska kromatografija - elementna masna spektrometrija za karakterizacijo organofosfornih spojin"; Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani
- Doktorat: mag. B. Podkrajšek, univ. dipl. kem.; naslov disertacije: "Vpliv mangana in karboksilnih kislin na oksidacijo žveplovih(IV) zvrsti v troposferski vodni fazi"; Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani; mentor: I. Grgić

POMEMBNI OBISKI / GOSTOVANJA

V tujino:
- B. Podkrajšek je bil na enomesečnem delovnem obisku pri prof. dr. H. Herrmannu na Oddelku za atmosfersko kemijo na Institute for Tropospheric Research, Leipzig, Nemčija
- J. Turšič je bila na dvo - tedenskem delovnem obisku na Inštitutu za eksperimentalno fiziko, Univerza na Dunaju, Avstrija
- M. Kovačevič je bil na eno - tedenskem delovnem obisku na Institute of Chemistry, Karl-Franzens University Graz, Avstrija
- S. Hočevar je bil na dvo - tedenskem delovnem obisku na Department of Analyti-

4500 PLUS) with the HPLC module and diode array spectrophotometric detector (Agilent, 1100 Series)
- Inductively coupled plasma atomic emission spectrometer (ICP-AES, Thermo Jarrell Ash, Model Atomscan 25) equipped with ultrasonic nebulizer (Cetac, Model U-6000 AT)
- Two ion chromatography (IC) systems with conductivity and spectrophotometric detection.
- Flow injection analyzer (ASIA Ismatec)
- Several modular electrochemical workstations (Autolab, Eco Chemie)
- Inverted optical microscope (Eclipse, Nikon)
- Microelectrode fabrication tools (capillary puller, 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)
- CHN/S Elemental analyzer (CE 440, Leeman Labs Inc.)
- Microwave oven for sample digestion (MLS 1200 MEGA, Milestone)

EDUCATION
- Ph.D.: M. Kovačevič, MSc; Thesis: "Application of hyphenated system liguid chromatography – element mass spectrometry for characterisation of organophosphorus compounds"; Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia
- Ph.D.: B. Podkrajšek, MSc; Thesis: "Influence of manganese and carboxylic acids on oxidation of sulphur(IV) species in tropospheric aqueous phase"; Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia; mentor: I. Grgić

IMPORTANT VISITS

Visits abroad:
- B. Podkrajšek: one month work visit to Prof. Dr. H. Herrmann at the Institute for Tropo-

cal Chemistry, University of Pardubice, Pardubice, Češka

- J. T. van Elteren je bil na eno - tedenskem delovnem obisku pri prof. Vanhaeckeju (Ghent University, Belgija) in dr. Masonu (Utrecht University, Nizozemska)
- J. T. van Elteren je bil na eno - tedenskem delovnem obisku pri prof. H. J. Glassu (Camborne School of Mines, University of Exeter, Velika Britanija)

Iz tujine:

- Prof. P. R. Haddad iz University of Tasmania, Hobart, Avstralija
- Dr. N. Avdalović iz Dionex Corporation, CA, ZDA
- P. Ctyroky iz Inštituta za eksperimentalno fiziko, Univerza na Dunaju, Avstrija, je bil na dvo - tedenskem delovnem obisku na Kemijskem inštitutu

spheric Research, Department for Atmospheric Chemistry, Leipzig, Germany

- J. Turšič: two - week work visit to the Institute for Experimental Physics, University of Vienna, Austria
- M. Kovačevič: one - week work visit to the Institute of Chemistry, Karl-Franzens University Graz, Austria
- S. Hočevar: two - week work visit to the Department of Analytical Chemistry, The University of Pardubice, Pardubice, Czech Republic
- J. T. van Elteren: one - week work visit to Prof. Vanhaecke (Ghent University, Belgium) and Dr. Mason (Utrecht University, The Netherlands)
- J. T. van Elteren: one - week visit to Prof. H. J. Glass (Camborne School of Mines, University of Exeter in Cornwall, UK)

Visits from abroad:

- Prof. P. R. Haddad from University of Tasmania, Hobart, Australia
- Dr. N. Avdalović from Dionex Corporation, CA, USA
- P. Ctyroky from the Institute for Experimental Physics, University of Vienna, Austria visited National Institute of Chemistry for two weeks

L05

Laboratorij za kemijo, biologijo in tehnologijo vod

Laboratory for Chemistry, Biology and Technology of Water

VODJA / HEAD
Prof. dr. Milenko Roš

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

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Anita Jemec

TEHNIČNO OSEBJE / TECHNICAL STAFF
Jelka Jelnikar
Emil Meden
Matjaž Omerzel

PRIPRAVNIKI / TRAINEES
Gizem Adal, Turčija / Turkey (IAESTE)

SLIKA 1
Šaržni biološki reaktor - preskus delovanja osnovnih delov laboratorijskega modela

FIGURE 1
Batch Reactor - test of basic parts of laboratory treatment plant

PODROČJA DEJAVNOSTI

a) Raziskovalni program

- Integralni pristop k preprečevanju onesnaževanja voda (MŠZŠ)

b) Raziskovalni projekti

- Razvoj temeljnih konceptov sledljivosti in merilne negotovosti v meroslovju v kemiji (MŠZŠ) - nosilka: dr. Andreja Drolc (do 30. 6. 2004)

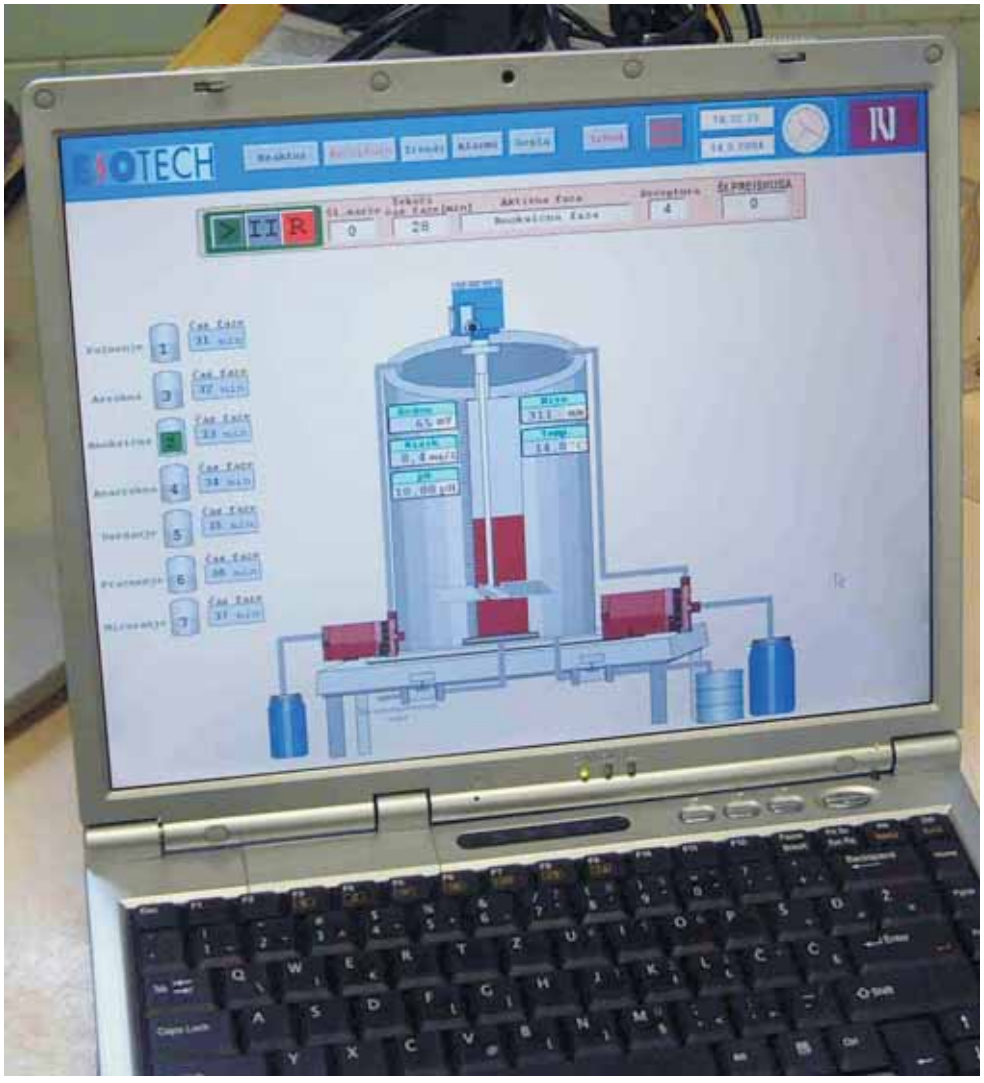
RESEARCH ACTIVITIES

a) Research Programme

- Integral approach to water pollution prevention

b) Research Projects

- Development of basic concepts of traceability and measurement uncertainty in metrology in chemistry (MŠZŠ) - principal researcher: A. Drolc, Ph. D. (till 30. June 2004)



SLIKA 2
Kontrolni sistem šaržnega biološkega reaktorja

FIGURE 2
Batch Reactor - research work with a real wastewater

- Meroslovna sledljivost v kemiji - vloga referenčnih materialov in referenčnih merjenj - nosilka: dr. Andreja Drolc (od 1. 7. 2004)
- Razvoj postopka za stabilizacijo, mineralizacijo in higienizacijo blata iz malih čistilnih naprav (MŠZŠ) - nosilec: dr. Gregor D. Zupančič (od 1. 7. 2004)
- Kemijsko in biološko sledenje neonukleotidov in njihovega vpliva v okolju (nosilka: doc. dr. Polonca Trebše, Politehnika Nova Gorica)
- Biološki testi za ugotavljanje toksičnosti in genotoksičnosti vode, zemlje in hrane (nosilka: prof. dr. Romana Marinšek Logar, Biotehniška fakulteta Univerze v Ljubljani)
- Razvoj celovitega sistema za ugotavljanje toksičnosti in genotoksičnosti v zemlji, vodi in hrani v soglasju s smernicami EU (nosilka: prof. dr. Romana Marinšek Logar, Biotehniška fakulteta Univerze v Ljubljani)

c) Slovenski ekološki grozd
- Sodelovali smo na projektih:

  Razvoj in avtomatizacija SBR in

  Raziskave mineralizacije blata iz bioloških čistilnih naprav na pilotni napravi

d) Center odličnosti - okoljske tehnologije
- Sodelovanje na pripravi projektov:

  Razvoj novih metod za čiščenje odpadnih vod v ŠBR in

  Biološka stabilizacija blata

BIBLIOGRAFIJA

6 izvirnih znanstvenih člankov
1 poljudni članek
1 samostojni znanstveni sestavek v monografiji
2 samostojna strokovna sestavka v monografijah
2 drugi učni gradivi
1 objavljeni znanstveni prispevek na konferenci (vabljeno predavanje)
3 objavljeni strokovni prispevki na konferencah (vabljeno predavanje)
5 objavljenih znanstvenih prispevkov na konferencah

- Metrological traceability in chemistry - role of reference materials and reference measurements (MŠZŠ) - principal researcher: A. Drolc, Ph. D. (since 1. July 2004)
- Procedure development for stabilization, mineralization and hygienization of sludge from small biological wastewater treatment plants (MŠZŠ) - principal researcher: Gregor D. Zupančič, Ph. D.
- Chemical and biological monitoring of neonicotinoids and their impact assessment in the environment (principal researcher: Prof. Polonca Trebše, Ph. D., Nova Gorica Politehnic, Slovenia)
- Biological tests for toxicity and genotoxicity determination in water, soil, and food (principal researcher: Prof. Romana Marinšek Logar, Ph. D., Biotehnical faculty, University of Ljubljana, Slovenia)
- Development of an integrated system for assessment of toxicity and genotoxicity in soil, water, and food in concordance with the EU directives (principal researcher: Prof. Romana Marinšek Logar, Ph. D., Biotehnical faculty, University of Ljubljana, Slovenia)

c) Slovenian Ecological Cluster
- Co - operation on the following sub - projects:
- Development and automation of SBR
- Research on mineralization of sludge from biological wastewater treatment plants

d) Centre of Excellence
- Co - operation on the following sub - projects:
- Development of new methods on wastewater treatment in the SBR
- Biological stabilization of sludge

BIBLIOGRAPHY

6 Original Scientific Articles
1 Popular Article
1 Scientific Article in a Monograph
2 Professional Articles in Monographs

21 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 objavljeni povzetek strokovnega prispevka na konferenci
1 patent
2 prispevka na konferencah brez natisa
10 končnih poročil o rezultatih raziskav
6 elaboratov, predštudij, študij
4 izvedenska mnenja
4 diplome
3 magisteriji
1 doktorat
1 uredništvo revije

GLAVNI DOSEŽKI V LETU 2004

- Priprava sistema za avtomatsko vodenje šaržnega biološkega reaktorja (v letu 2005 bo sistem realiziral ESOTECH)
- Raziskave na področju mineralizacije blata iz bioloških čistilnih naprav s čistim kisikom in patent s področja mineralizacije blata
- Vzdrževanje akreditacije po standardu SIST EN ISO/IEC 17025
- Priprava metode za določevanje organskih spojin v vodnih vzorcih na GC-MS
- Urad za meroslovje Republike Slovenije (MIRS) je Laboratorij za kemijo, biologijo in tehnologijo vod imenoval za nosilca referenčnega etalona enote za MOL (področje varovanje okolja, vrsta vzorca odpadne vode)
- TrainMic Training of Trainers, EC-DG JRC-IRMM
- Uporaba naše tehnologije pri postavitvi čistilnih naprav Slavkov dom (25 PE), Dotik (25 PE), Rotar Trboje (25 PE)

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Nuklearna elektrarna Krško, Krško
- Esotech d.d., Velenje
- Dr. Duhovnik d.o.o., Seničica
- Cinkarna, Celje
- Bayer farma d.o.o, Ljubljana

2 Other Educational Materials
1 Published Scientific Conference Contribution (Invited Lecture)
3 Published Professional Conference Contributions (Invited Lecture)
5 Published Scientific Conference Contributions
21 Published Scientific Conference Contribution Abstracts
1 Published Professional Conference Contribution Abstract
1 Patent
2 Unpublished Conference Contributions
10 Final Research Reports
6 Treatises, Preliminary Studies, Studies
4 Expert Opinions
4 Undergraduate Theses
3 Master's Theses
1 Doctoral Dissertation
1 Editorship

IMPORTANT ACHIEVEMENTS IN 2004

- Project of autoimmunization of laboratory scale of the SBR
- Research of mineralization of excess biological sludge with pure oxygen
- Support of accreditation according to standard SIST EN ISO/IEC 17025
- Preparation of the method for determination of organic compounds in water samples on GC-MS
- Holder of national reference etalon of "mole" (area protection of environment, sample type waste water), based on authorisation of Metrological institute of republic of Slovenia (MIRS)
- TrainMic Training of Trainers, EC-DG JRC-IRMM
- Application of our technology at new wastewater treatment plants Slavkov dom (25 PE), Dotik (25 PE), Rotar Trboje (25 PE)

SLIKA 3
Šaržni biološki reaktor - raziskave z realno odpadno vodo

FIGURE 3
Sequencing Batch Reactor - research work with a real wastewater

- Krka d.d., Novo mesto
- JP Energetika KEL, Ljubljana
- Schaeffer Consult, Straža
- CČN Domžale - Kamnik, Domžale
- Komunalno podjetje Velenje, Koroška 37B, Velenje

MEDNARODNO SODELOVANJE
- MESSER GRIESHEIM GMBH, Nemčija (Pure Oxygen Aerobic Digestion of Sludge)
- CoEPT (The Comparison of the Operating Protocols of European Proficiency Testing Scheme)
- JRC-IRMM (mednarodne delavnice TrainMiC - Training of Metrology in Chemistry)

POMEMBNI INŠTRUMENTI IN OPREMA
- Štirje kombinirani anaerobno-anoksično-aerobni reaktorji (KI)
- Avtomatizirani šaržni biološki reaktor (ŠBR)
- LUMIS-TOX aparatura (dr. Lange)
- Avtomatizirani respirometer (MICRO-Oxymax 6.0, Columbus Instruments)
- Ionski kromatograf (DIONEX 120) s samodejnim vzorčevalnikom (DIONEX AS 3500)
- Kjeltec sistem 2300 Autosystem II (FOSS Tecator) za razklop in določanje Kjeldahlovega dušika
- TOC analizator TOC-5000A (SHIMADZU)
- Laboratorijski modeli rek
- Spektrofotometer Lambda 20 (Perkin-Elmer)
- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector
- Štirje laboratorijski modeli bioloških čistilnih naprav

IZOBRAŽEVANJE
- Izvajanje diplomskih del, ki jih vodi prof. dr. Jana Zagorc Končan in prof. dr. Milenko Roš
- Izvajanje vaj za FKKT, ki jih vodi prof. dr. Jana Zagorc Končan, habilitirani za vodenje vaj pa

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS
- Nuclear Power Plant, Krško, Slovenia
- Esotech d.d., Velenje, Slovenia
- Cinkarna, Celje, Slovenia
- Dr. Duhovnik d.o.o., Seničica, Slovenia
- Bayer Farm, Ljubljana, Slovenia
- Krka d.d., Novo mesto, Slovenia
- JP Energetika, KEL Ljubljana, Slovenia
- Schaeffer Consult, Straža, Slovenia
- Central WWTP Domžale - Kamnik, Domžale, Slovenia
- Municipality of Velenje, Koroška 37B, Velenje, Slovenia

INTERNATIONAL COLLABORATION
- MESSER GRIESHEIM GMBH, Griesheim, Germany
- CoEPT (The Comparison of the Operating Protocols of European Proficiency Testing Scheme)
- JRC-IRMM (international workshops TrainMiC - Training of Metrology in Chemistry)

MAJOR EQUIPMENT
- Four combined anaerobic-anoxic-aerobic reactors
- Automated sequencing batch reactor (SBR)
- LUMIS-TOX apparatus (Dr. Lange)
- Automated respirometer (MICRO-Oxymax 6.0, Columbus Instruments)
- Ion chromatograph (DIONEX 120) with automatic sampler (DIONEX AS 3500)
- Kjeltec system 2300 Autosystem II (FOSS Tecator) for Kjeldahl N determination
- TOC-5000A, SHIMADZU for determination of Total Organic Carbon (TOC)
- Laboratory river models
- Spectrophotometer Lambda 20 (Perkin-Elmer)

sta tudi dr. Andreja Drolc in dr. Magda Cotman

- Soorganizacija delavnice TrainMic, skupaj z JRC-IRMM iz Belgije
- Soorganizacija konference Vodni dnevi 2004, kjer so sodelovali kot predavatelji tudi sodelavci L05
- Sodelovanje pri organizaciji mednarodnega kongresa Life Sciences 04, Nova Gorica ter sodelovanje raziskovalcev L05 s predstavitvijo znanstvenih prispevkov na konferenci
- Sodelovanje pri izvedbi diplomskih in doktorskih del z Biotehniško fakulteto Univerze v Ljubljani, Oddelek za zootehniko in Oddelek za biologijo

- Agilent Technologies 6890 N GC System + 5973 Mass selective Detector
- Four laboratory scale aerobic wastewater treatment plants

EDUCATION

- Carrying out of diloma works, master's works and doctoral thesis conducted by Prof. Dr. Jana Zagorc Končan and Prof. Dr. Milenko Roš
- Practice performing for the Faculty of Chemistry and Chemical Technology (Chemical engineering, Environmental protection) conducted by Prof. Dr. Jana Zagorc Končan, assistants for practice are also Dr. Andreja Drolc and Dr. Magda Cotman
- Train MIc workshop organization in collaboration with JRC-IRMM, Belgium
- Co - organization of the Conference WATER DAYS 2004
- Co - organisation of the International Conference Life Sciences 04, Nova Gorica, Slovenia and presentation of the research work at the Conference
- Cooperation with Biotechnical faculty, University of Ljubljana, Zootechnical Department and Department of Biology in undergraduate and postgraduate theses

L06

Laboratorij za prehrambeno kemijo

Laboratory for Food Chemistry

VODJA / HEAD
Dr. Mirko Prošek

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

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Brigita Lapornik
Mitja Križman
Kajetan Trošt
Maja Fir

TEHNIČNO OSEBJE / TECHNICAL STAFF
Mateja Puklavec

PRIPRAVNIKI / TRAINEES
Tina Celestina

PODROČJA DEJAVNOSTI

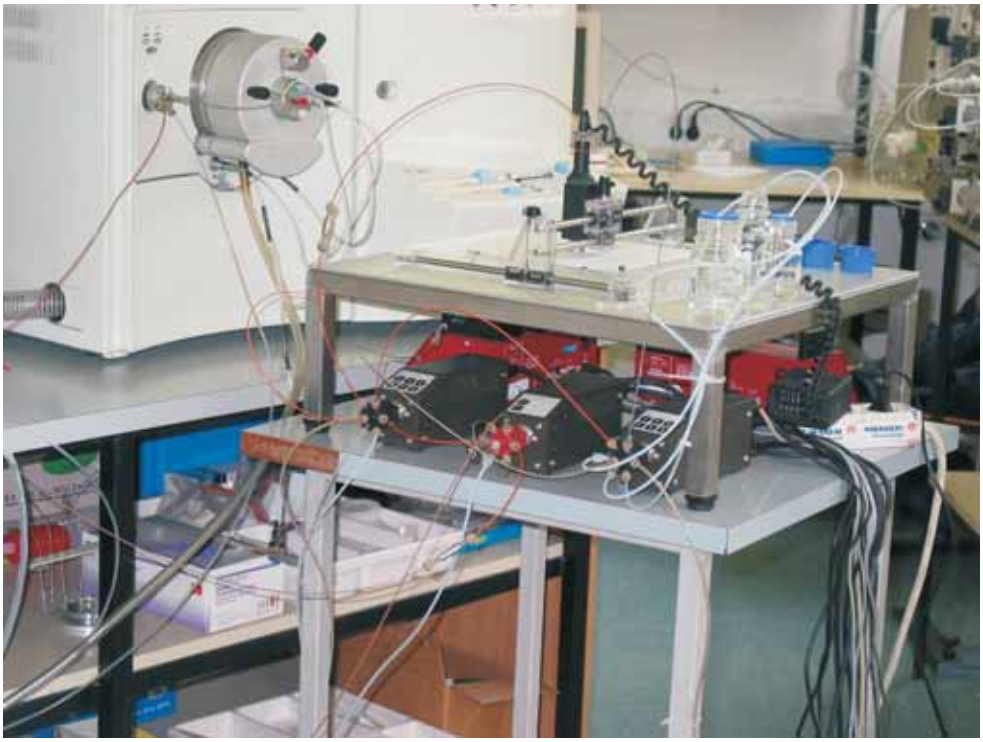
Raziskovalno delo Laboratorija za prehrambeno kemijo je usmerjeno na področje znanstvenega načrtovanja izdelkov za zdravo prehrano. Delo poteka v petih podskupinah in sicer na:

- določanju spojin naravnega izvora s sodobnimi kromatografskimi in spektroskopskimi tehnikami;
- razvoju novih prehrambenih izdelkov in prehranskih dodatkov s funkcionalnimi lastnostmi;
- preprečevanju kemijskih tveganj z upoštevanjem dobrih praks (GLP in GMP) pri razvoju in validaciji analiznih metod, tehnološke validacije, validacije čiščenja in HCCAPa;
- pripravi in vrednotenju specialne prehrane (prehrambeni inženering);

RESEARCH ACTIVITIES

Research Activities in the Laboratory for Food Chemistry are oriented into the Scientifically designed food for healthy nutrition, and they are divided in five main research and development fields:

- Investigation of compounds from natural sources by modern chromatographic and spectroscopic techniques;
- Development of new food products and food additives with functional activities;
- Minimization of chemical hazard in food production according to GLP, GMP, at method validations, technical validations, cleaning validations and HCCAP;
- Evaluation of special food and food engineering;



SLIKA 1
Razvoj novega sistema za in-line TLC-MS analizo

FIGURE 1
Development of new in-line TLC-MS system

- razvoju in validaciji novih analiznih metod in analiznih tehnik.

BIBLIOGRAFIJA

7 izvirnih znanstvenih člankov
1 strokovni članek
1 poljudni članek
6 objavljenih znanstvenih prispevkov na konferencah
20 objavljenih povzetkov znanstvenih prispevkov na konferencah
2 patentni prijavi
1 diploma
1 doktorat

GLAVNI DOSEŽKI V LETU 2004

- Raziskave so potekale na področju prehrambene in analizne kemije ter razvoju novih farmacevtskih izdelkov in učinkovin. Razvoj-

- Development and validation of new analytical techniques and methods.

BIBLIOGRAPHY

7 Original Scientific Articles
1 Professional Article
1 Popular Article
6 Published Scientific Conference Contributions
20 Published Scientific Conference Contribution Abstracts
2 Patent Applications
1 Undergraduate Thesis
1 Doctoral Dissertation

IMPORTANT ACHIEVEMENTS IN 2004

Research activities in L06 were focused on preparation and characterization of new food

SLIKA 2
Patentirani sušilnik za TLC plošče, razvit na Kemijskem intitutu

FIGURE 2
Patented TLC-dryer, developed on National Institute of Chemistry

no raziskovalne naloge so vezane na razvoj, optimizacijo, validacijo in uporabo analiznih tehnik in metod.

- Pri vrednotenju prehrambenih in farmacevstkih izdelkov, kakor tudi pri zasledovanju aktivnih komponent v bioloških poizkusih, smo zelo uspešno uporabljali separacijske in spektroskopske analizne tehnike in njihove kombinacije.
- Skupaj s sodelavci tehnične službe smo v delavnicah Kemijskega inštituta izdelali prvo komercialno serijo sušilnikov za TLC plošče. Izdelek je bil preizkušen v analiznih laboratorijih nekaterih slovenskih farmacevtskih tovarn. Dobil je zelo pohvalne ocene, ker istočasno izboljša ponovljivost analiznih meritev in poveča požarno varnost, ker omogoča sušenje v zaprtih in kontroliranih pogojih. Izdelek ima slovenski patent in je v fazi patentiranja v nekaterih evropskih državah.
- V sodelovanju z zunanjimi raziskovalnimi institucijami in preko lastnih projektov smo ovrednotili nekatere učinkovine rastlinskega in živalskega izvora, pomembne za človekovo zdravje.
- Razvili in validirali smo analizne metode za kvantitativno vrednotenje holesterola, raznih antioksidantov, vitaminiov, provitaminovi itd. Razvili smo originalno HPLC/MS metodo za določevanje aloina in koencima CoQ10 v prehrambenih in farmacevtskih izdelkih.
- Razvili smo postopek priprave kompleksa (vključka) CoQ10 z β-ciklodekstrinom. Sintetizirani kompleks, ki je za razliko od originalne substance vodotopen, lahko uporabljamo kot prehrambeni dodatek v raznih prehrambenih izdelkih. Pripravili smo mleko, jogurt, sadne sokove in celo mineralno vodo obogateno z CoQ10. Izdelke smo kemijsko in organoleptično testirali in sedaj pričakujemo, da se bodo kmalu pojavil v redni prodaji. Za razviti postopek smo vložili tudi patentno prijavo.

products, development and optimization of new analytical techniques.

- Together with the Technical department of National Institute of Chemistry we constructed and produced a new type of TLC dryer. Instrument was tested in analytical laboratories of some Slovenian pharmaceutical factories. It was accepted very well, because it doesn't improve only the quality of analytical measurements but also offers safe drying conditions. Instrument is patented in Slovenia and in some European countries.
- Validation and quantification of food and pharmaceutical products (ingredients) together with determination of levels of active substances were very successfully performed with combinations of chromatography with mass spectrometry. We developed and validated different analytical methods for quantitative determination of cholesterol, antioxidants vitamins and provitamins. New original HPLC/MS analytical methods for quantitative evaluation of aloine and coenzyme Q10 in food and pharmaceutical products were prepared.
- We developed and patented new water-soluble form of the CoQ10-βCD complex. Prepared complex is used as a food additive in a different type of products, for instance in milk, yogurt, juices, and even in mineral waters. Chemical and organoleptic tests were very positive and we are now trying to organize production of food products will increased amount of CoQ10.
- Studies of vegetable oils were focused on preparation and chemical characterisation of new food additives with antioxidant activities. Our additives control the oxidation of oils and products with certain amount of fat (mayonnaises, cream, milk etc.) at higher temperatures and during storage time.
- Our activities within the European project TOM were focused on the identification and isolation of antioxidants, enzymes and other compounds from the solid residue of the to-

- Na področju jedilnih olj smo pripravili in ovrednotili nekatere nove prehranske dodatke z antioksidacijskimi lastnostmi, ki pri termični obdelavi in skladiščenju preprečujejo oksidacijski razpad. Pričakujemo, da bodo te učinkovine zagotavljale kontrolirano stabilnost olj in drugih izdelkih na bazi maščob (majoneze, smetana, mleko, itd).
- Dokončali smo postopek za optimalno izolacijo fenolnih spojin iz specifičnih ostankov pri predelavi sadja, kot so grozdje, črni in rdeči ribez idr. Postopek je enostaven, cenen in ne vključuje zdravju škodljivih snovi. Pripravljeni prehranski dodatek z antioksidativnim delovanjem smo uporabili za izboljševanje organoleptičnih in prehrambenih lastnost v sadnih sokovih. Za pripravo in uporabo našega izdelka smo prejeli slovenski patent in se dogovarjamo za industrijsko uporabo.
- V okviru EU projekta TOM so bile naše raziskave usmerjene na področje izolacije antioksidantov, encimov in drugih spojin iz odpadkov iz proizvodnje izdelkov iz paradižnika. V sodelovanju s partnerji smo iz suhih olupkov ekstrahirali likopen. Razvili smo HPLC metodo za določanje cis in trans likopena in drugih karotenoidov prisotnih v različnih ekstraktih iz paradižnikovih olupkov. Poleg tega smo razvili nov postopek ekstrakcije in izolacije dveh encimov pektin metilesteraze (PME) in poligalakturonaze (PG) iz paradižnika. Za izolacijo so bili ključnega pomena CIM diski podjetja BIA Separations d.o.o., Ljubljana. Izolirana encima PME in PG bo nizozemsko podjetje Catchmabs uporabilo za generiranje monoklonskih protiteles iMab.
- S partnerji iz University of Helsinki, Finska smo testirali prototip multifunkcionalnega instrumenta (ExtraChrom®), s katerim smo izvedli ekstrakcijo hrastovega lubja in frakcionacijo ekstrakta. Zanimala nas je biološka aktivnost ekstraktov in frakcij, hkrati pa smo poskušali tudi identificirati čim več sestavin z zdravilnim učinkom, za kar smo

mato processing industry. In collaboration with project partners we obtained different extracts containing lycopene from tomato peels. We developed HPLC method for determination of cis and trans lycopene and other carotenoids in different extracts from tomato peels. We developed the extraction, isolation and purification procedure for isolation of the enzyme pectin methylesterase (PME) and polygalacturonase (PG) from tomato fruit. Purified PME and PG will be used by Catchmabs as target for the iMab generation.

- The main activity within the cooperation with the group from University of Helsinki, Finland was to use the multifunctional ExtraChrom® instrument for extraction of oak bark, and fractionation of the obtained extracts. We were interested in biologically active compounds and their identification by HPLC-MS. Although, the composition is rather complex, we succeed to identify some known biologically active substances.
- Additionally, we studied the potential of microcrystalline cellulose as sorbent in the separation of eight polyphenolic compounds: (+)-catechin, (-)-epicatechin, (-)-gallocatechin, (-)-epigallocatechin, (-)-epicatechin gallate, (-)-epigallocatechin gallate, procyanidin B1 and procyanidin B2. These compounds that have been shown to exhibit a wide variety of beneficial effects on human health and are also the building blocks of oligomeric procyanidins (condensed tannins). The applicability of the four newly proposed developing solvent systems were for the determination of these compounds on the cellulose HPTLC plates was confirmed by analysis of green tea and oak bark extracts.
- In the frame of cooperation with the group from Palacky University, Czech Republic (Faculty of Medicine, Institute of Medical Chemistry and Biochemistry) we characterised some biologically active compounds from tubers and leaves of Yacon (Smallanthus sonchi-

uporabili HPLC-MS. Ugotovili smo, da je sestava zelo kompleksna, kljub temu pa smo uspeli dokazati prisotnost nekaj znanih biološko aktivnih spojin. Raziskovali smo potencial mikrokristalinične celuloze kot sorbenta za ločbo osmih spojin: (+)-katehin, (-)-epicatehin, (-)-galokatehin, (-)-epigalokatehin, (-)-epikatehin galat, (-)-epigalokatehin galat, procianidin B1 in procianidin B2. Gre za spojine z dokazano biološko aktivnostijo, ki so tudi sestavni deli oligomernih procianidinov (kondenziranih taninov). Razvili smo štiri nove sisteme za določanje flavan-3-olov na HPTLC ploščah s celuloznim sorbentom. Uporabnost teh sistemov v praksi smo potrdili z ekstrakti zelenega čaja in hrastovega lubja.

- V sodelovanju s partnerji s Palacky University, Faculty of Medicine, Institute of Medical Chemistry and Biochemistry, Češka, smo nadaljevali s karakterizacijo biološko aktivnih spojin iz listov in gomoljev jakuna (Smallanthus sonchifolius), ki naj bi imele ugoden vpliv na zdravje in počutje in naj bi ščitile pred pojavi nekaterih kroničnih degenerativnih obolenj. S tankoplastno kromatografijo (analizno in preparativno TLC) in s tekočinsko kromatografijo visoke ločljivosti z masnim detektorjem (HPLC-MS) smo v ekstraktih prvi dokazali prisotnost desetih fenolnih kislin v listih in šestih fenolnih kislin v gomoljih jakuna. S TLC in HPLC-MS smo dokazali visoko vsebnost ß-1,2-oligofruktanov v gomoljih jakuna. Poleg tega smo znanstveno ovrednotili različne ekstrakte gomoljev in listov jakuna ovrednotili glede na sposobnost vezanja prostih radikalov, zaščite celic in vpliva na celični metabolizem ogljikovih hidratov.
- V okviru sodelovanja s skupino z University of Belgrade, Faculty of Pharmacy, Srbija in Črna gora smo testirali monolitni sorbent (Merck, Nemčija), ki predstavlja novo generacijo sorbentov na področju tankoplastne kromatografije. Gre za miniaturne UTLC ("ultra - thin-layer chromatography")

folius). Those compounds could be used as active ingredients in dietary supplements with preventive effects against some chronic diseases. Our investigation of the extracts using thin-layer chromatography (TLC) and high performance liquid chromatography with mass spectrometric detector (HPLC-MS) showed that yacon is a rich source of phenolic acids and other radical scavenging compounds. We found ten newly discovered phenolic acids in the leaves and six phenolic acid in the tubers of yacon. Additionally, using TLC and HPLC-MS we proved high content of ß-1,2-oligofructans in the tubers. Various extracts prepared from the tubers, and aerial part were investigated for biological activity (antiradical, antioxidant, cytoprotective activity and influence on cellular carbohydrate metabolism).

- In the frame of cooperation with the group from University of Belgrade, Serbia and Montenegro (Faculty of Pharmacy) we tested monolithic sorbent (Merck, Germany), which represents a new generation of the sorbents in the field of thin-layer chromatography. This sorbent is used for UTLC ("ultra - thin-layer chromatography") plates with the size 6 x 3,6 mm. The thickness of the sorbent layer is 10 μm. To compare the features of HPTLC and UTLC plates we developed a new method, which enables the separation of six compounds from the group of ACE inhibitors on the same HPTLC plate. Due to the fact that chromatographic chambers for optimal development of so small plates are not commercially available, we made an adapter for development of UTLC plates in horizontal developing chamber.
- Within the cooperation with the group from University Medical Centre Ljubljana, Slovenia we investigated the influence of enteral nutrition on the treatment of multiple injured patients. Intestinal permeability was determined by using our method, which enabled us to determine lactulose and mannitol in 66

plošče velikosti 6 x 3,6 mm, ki imajo le 10 μm sloj sorbenta. Da bi lahko primerjali HPTLC in UTLC plošče na isti aplikaciji, smo najprej razvili metodo, ki omogoča ločbo šestih spojin (zdravil) iz skupine ACE inhibitorjev na HPTLC plošči. Ker še vedno niso komercialno dostopne kadi za razvijanje tako majhnih plošč, smo naredili adapter za razvijanje UTLC plošč v horizontalni kadi.

- V sodelovanju s skupino s Kliničnega centra smo raziskovali vpliv enteralnega hranjenja na zdravljenje politravmatiziranih poškodovancev. Za študij povezave med propustnostjo črevesne stene in odpovedovanjem organskih sistemov smo s TLC analizno metodo (razvito leta 2003), ki omogoča določanje laktuloze in manitola v vzorcih urina na isti HPTLC plošči, analizirali 66 vzorcev urina.
- Kot odgovorni nosilci smo v CVTA sodelovali pri načrtovanju in izvedbi številnih študij, kakor tudi pri validaciji analiznih metod, postopkov čiščenja in tehnoloških validacijah. Razvili smo več novih TLC analiznih metod za določanje ostankov farmacevtskih učinkovin na proizvodni opremi, ki smo jih tudi validirali.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

Sodelovanje je potekalo s številnimi slovenskimi podjetji kot so Lek d.d., Ljubljana; Krka d.d., Novo mesto; Bayer Pharma d.o.o., Ljubljana; Kolinska d.d., Ljubljana; Fructal d.d., Ajdovščina; Pivovarna Union d.d., Ljubljana; BIA Separations d.o.o., Ljubljana in institucijami kot so, Klinični center Ljubljana; Veterinarska fakulteta, Univerza v Ljubljani; Veterinarska klinika, Ljubljana; Zavod za zdravstveno varstvo Maribor; Biotehnična fakulteta, Univerza v Ljubljani; Inštitut za varovanje zdravja, Ljubljana.

MEDNARODNO SODELOVANJE

Evropska projekta:

- Sodelovanje pri Evropskem centru odličnosti,

urine samples on the same amino HPTLC plate. The ratio of lactulose/mannitol excretion in urine after their administration is of great importance for evaluation of malabsorption and intestinal permeability disruption in some diseases.

- The new procedure for preparation of the food additive with antioxidant activities especially suitable for fruit juices was patented. Our product consist of antocianins isolated from grape, black and red currant skin and juice.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

Cooperation was going on with pharmaceutical and food factories: Lek d.d., Ljubljana, Slovenia; Krka d.d., Novo mesto Slovenia; Bayer Pharma d.o.o., Ljubljana, Slovenia; Kolinska d.d., Ljubljana, Slovenia; Fructal d.d., Ajdovščina, Slovenia; Pivovarna Union d.d., Ljubljana, Slovenia; BIA Separations d.o.o., Ljubljana, Slovenia; Medical Centre Ljubljana, Slovenia etc.

INTERNATIONAL COLLABORATION

European projects:

- Participation with a workpackage (WP-11) at European centre of excellence: "Use of NMR spectroscopy in combination with computational methods on systems with biological interest", 5th Framework Programme, contract no. ICA1-CT-2000-70034; SLONMR (WP-11: "Drug discovery from natural products")
- CRAFT: "Development of new food additives extracted from the solid residue of tomato processing industry for the application in functional food" (5th Framework Programme, QLK1-CT-2002-71361, TOM)

Bilateral projects:

- Slovenia - Czech Republic: "Biologicaly active compounds from tubers and leaves of Yacon (Smallanthus sonchifolius)" with Palacky University, Faculty of Medicine, In-

5. okvirni program EU, pogodba št. ICA1-CT-2000-70034 ("Work package" WP-11: "Drug discovery from natural products")

- CRAFT: "Development of new food additives extracted from the solid residue of tomato processing industry for the application in functional food" (5. okvirni program EU, QLK1-CT-2002-71361, TOM)

Bilateralna projekta:

- Slovenija - Češka: s Palacky University, Faculty of Medicine, Institute of Medicinal Chemistry and Biochemistry (Olomouc, Češka): "Biologicaly active compounds from tubers and leaves of Yacon (Smallanthus sonchifolius)", nosilki: dr. Irena Vovk in prof. dr. Jitka Ulrichova
- Slovenija - Srbija in Črna gora: z University of Belgrade, Faculty of Pharmacy (Beograd, Srbija in Črna gora): "Kromatografske metode v analizi farmakološko aktivnih substanc, proučevanje korelacije strukture teh substanc s fizikalno kemijskimi lastnostmi (QSPR) ter z njihovo biološko aktivnostjo (QSAR)", nosilki: dr. Irena Vovk in prof. dr. Danica Agbaba

Inštitucije:

- Palacky University, Faculty of Medicine, Institute of Medicinal Chemistry and Biochemistry, Olomuc, Češka
- Technology Transfer Centre, Bremerhaven, Nemčija
- Catchmabs, Wageningen, Nizozemska
- Fundation Azti, Španija
- Potato research institute, Havlickuv Brod, Češka
- University of Belgrade, Faculty of Pharmacy, Beograd, Srbija in Črna gora
- University of Helsinki, Faculty of Pharmacy, Helsinki, Finska
- Research Institute for Chromatography, Kortrijk, Belgija

stitute of Medicinal Chemistry and Biochemistry (Olomouc, Czech Republic); principal researchers: Dr. Irena Vovk and Prof. Dr. Jitka Ulrichova

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

Institutions:

- Palacky University, Faculty of Medicine, Institute of Medicinal Chemistry and Biochemistry, Olomuc, Czech Republic
- Technology Transfer Centre, Bremerhaven, Germany
- Catchmabs, Wageningen, The Netherlands
- Fundation Azti, Spain
- Potato research institute, Havlickuv Brod, Czech Republic
- University of Belgrade, Faculty of Pharmacy, Serbia and Montenegro
- University of Helsinki, Faculty of Pharmacy, Finland
- Research Institute for Chromatography, Kortrijk, Belgium

MAJOR EQUIPMENT

- 5 HPLC systems
- HPLC/MS
- TLC (TLC/MS)
- CE
- GC (4 sytems)

POMEMBNI INŠTRUMENTI IN OPREMA

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

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

L07

Laboratorij za polimerno kemijo in tehnologijo

Laboratory for Polymer Chemistry and Technology

VODJA / HEAD
Doc. dr. Majda Žigon

RAZISKOVALCI / RESEARCHERS
Dr. Gabriela Ambrožič
Dr. Alojz Anžlovar
Dr. Miroslav Huskić
Dr. Andrej Kržan
Doc. dr. Matjaž Kunaver
Dr. Ida Mav Golež
Dr. Ema Žagar

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Nada Verdel (do / until 30. 6. 2004)
Maja Gričar (od / since 1. 10. 2004)

TEHNIČNO OSEBJE / TECHNICAL STAFF
Miran Lavrič
Mira Mikuž
Polona Prosen
Mirjana Širca

PRIPRAVNIKI / TRAINEES
Maja Gričar (1. 1. - 30. 9.)

PODROČJA DEJAVNOSTI

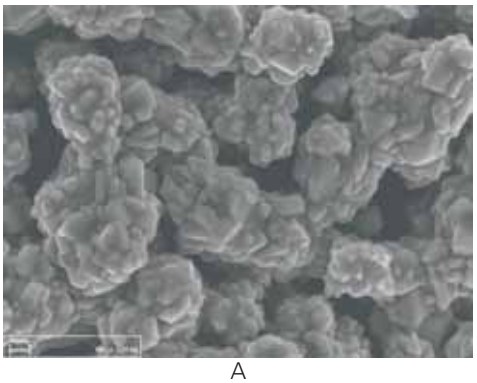
Raziskave so potekale v okviru raziskovalnega programa P2-0145-0104 (Polimeri s posebnimi lastnostmi), treh podoktorskih projektov, štirih aplikativnih projektov (od teh eden v sodelovanju z L02, eden s Fakulteto za farmacijo Univerze v Ljubljani in eden z Institutom Jožef Stefan, Ljubljana), dveh evropskih projektov, evropske mreže odličnosti, treh bilateralnih projektov in projektov za naročnike. Področja dejavnosti L07 so:

- Stranskoverižni poliestri in poliuretani
- Delno prepletene polimerne mreže iz funkcionaliziranih poliuretanskih in polimetakrilatnih predpolimerov
- Prevodni polimeri na osnovi substituiranih polianilinov in kompozitne polimerne membrane iz temperaturno obstojnih polimerov s polarnimi nosilci naboja
- Biorazgradljivi polimeri
- Modificirani nanodelci, polimerni nanokompoziti
- Kemijska razgradnja naravnih in umetnih polimerov
- Lastnosti polimerov in polimernih materialov

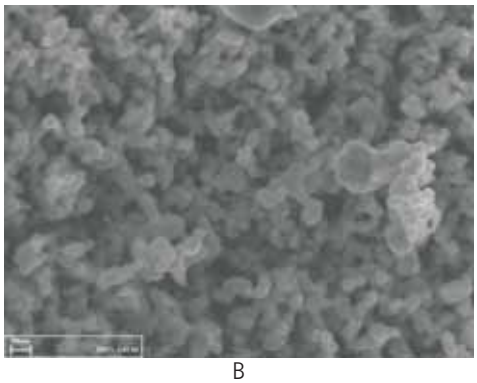
RESEARCH ACTIVITIES

Research was conducted in the frame of the research Programme P2-0145-0104 (Specialty Polymers), three post-doc projects, four applied projects (in collaboration with L02, the Faculty of Pharmacy of the University of Ljubljana, Slovenia, and Jožef Stefan Institute, Ljubljana, Slovenia), two European projects (5. FP), European Network of Excellence (6. FP), three bilateral research projects, and projects with industrial partners. The research activities of L07 are:

- Side-chain polyesters and polyurethanes
- Semi-interpenetrating polymer networks based on functionalized polyurethane and polymethacrylate prepolymers
- Conductive polymers based on substituted polyanilines and composite polymer membranes made of thermally resistant polymers with polar charge carriers
- Biodegradable polymers
- Modified nanoparticles, polymer-based nanocomposites
- Chemical degradation of natural and synthetic polymers



A



B

SLIKA

Vrstične elektronske mikrografije delcev kovinskega bakra, reduciranih v dietilen glikolu pri 220°C (povečava – 500000x): a) dietilen glikol brez dodatkov, b) dietilen glikol z dodatkom zaščitnega polimernega koloida – poli(vinil pirolidona)

FIGURE

SEM micrographs of metallic copper particles reduced in di(ethylene glycol) at 220°C (magnification – 500000x): a) pure di(ethylene glycol), b) di(ethylene glycol) with added polymer protective colloid – poly(vinyl pyrrolidone)

- Razvojne raziskave in storitve, predvsem na področju veziv, termoplastov in recikliranja industrijskega polimernega odpadka
- Analiza in karakterizacija komercialnih polimerov s spektroskopskimi (FTIR, NMR), kromatografskimi (GC, GC-MS, IGC, SEC, SEC-MALS) in termičnimi (DSC) metodami za naročnike

BIBLIOGRAFIJA

11 izvirnih znanstvenih člankov
2 strokovna članka
2 poljudna članka
1 drugi članek in sestavek
3 objavljeni znanstveni prispevki na konferencah
2 objavljena strokovna prispevka na konferencah
17 objavljenih povzetkov znanstvenih prispevkov na konferencah
4 patentne prijave
2 prispevka na konferenci brez natisa
3 končna poročila o rezultatih raziskav
1 diploma
1 doktorat
4 uredništva revij

GLAVNI DOSEŽKI V LETU 2004

- Pripravili smo stranskoverižne poliestre z nitroazobenzenskimi in / ali metoksi-azobenzenskimi mezogenimi enotami na diolni (dietanolamin) in kislinski komponenti (dimetiletilester hidroksi-*izo*-ftalne kisline) z različno dolžino gibljive alkilne verige. Poliestri so kristalinični, amorfni ali tekočekristalinični.
- Z ESR spektroskopijo spinsko označene polimetakrilatne komponente smo raziskali vpliv interakcij med komplementarnimi funkcionalnimi skupinami poliestrskega poliuretana in polimetakrilata na heterogenost segmentnega gibanja in na fazne prehode delno prepletenih polimernih mrež. Pri mejni koncentraciji funkcionalnih skupin 0,25 mmol g^{-1} segmentno gibanje postane manj ovirano, kar smo pripisali spremembam lokalne gostote zlaganja verig in strukture.

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

BIBLIOGRAPHY

11 Original Scientific Articles
2 Professional Articles
2 Popular Articles
1 Other Article
3 Published Scientific Conference Contributions
2 Published Professional Conference Contributions
17 Published Scientific Conference Contribution Abstracts
4 Patent Applications
2 Unpublished Conference Contributions
3 Final Research Reports
1 Undergraduate Thesis
1 Doctoral Dissertation
4 Editorships

IMPORTANT ACHIEVEMENTS IN 2004

- We prepared side-chain polyesters with a nitroazobenzene and / or methoxyzobenzene mesogenic groups attached to diol (diethanolamine) and acid component (dimethyl ester of hydroxy-*iso*-phtalic acid) with various aliphatic spacer lengths. Depending on their composition, amorphous, crystalline or liquid crystalline polyesters were obtained.
- Using electron spin resonance (ESR) and spin labelled polymethacrylic (PM) components we investigated the influence of interactions between complementary functional groups of polyester polyurethane and PM component on the heterogeneity of segmental motion and transitions of semi-interpenetrated polymer networks. Restriction of segmental

- Polianilin in kopolimere 2- in 3- substituiranih anilinov smo dopirali z 1M HCl, z večjimi protonskimi kislinami (oksalna kislina, p-toluensulfonska kislina, 5-sulfosalicilna kislina, HClO4) in polimernim dopantom poliakrilno kislino. Filmi dopiranih substituiranih polianilinov so imeli nekoliko slabše mehanske lastnosti in večjo prevodnost kot dedopirani PANI.
- Nadaljevali smo z razvojem protonsko prevodnih polimernih membran (sodelovanje z L13) na osnovi fluoriranega polimera in organsko anorganskih polnil. V zadnji fazi projekta smo opravili optimizacijo sestave in korelacijo sestave z ionsko prevodnostjo ter raziskali osnovne metode izdelave eno - in več - slojnih membran.
- Nove so raziskave polimernih nanokompozitov z modificiranim montmorilonitom (MMT). MMT je plastovit alumosilikat s šibko vezanimi ioni natrija ali kalcija, ki mu z zamenjavo s kvarternimi amonijevimi solmi spremenimo polarnost površine plasti in omogočimo pripravo polimernih nanokompozitov. MMT smo modificirali s tekočekristaliničnimi kvarternimi amonijevimi solmi in z *in situ* polimerizacijo v raztopini pripravili tekočekristalinične poliesterske nanokompozite. Pri polimerizaciji pride do vrivanja molekul polimera med plasti MMT.
- Po poliolnem postopku smo pripravili delce bakrovega (I) oksida in kovinskega Cu iz Cu (II) acetata ali Cu acetilacetonata (sodelovanje z L02). V dietilenglikolu redukcija do bakra poteče pri temperaturah nad 190°C, v 1,2-propilenglikolu pa nad 175°C. Velikost delcev je reda velikosti 100 nm in narašča z naraščanjem koncentracije izhodne spojine. Dodatek polimernega zaščitnega koloida polivinilpirolidona ali polimetakrilne kisline prepreči aglomeriranje Cu delcev in zniža njihovo velikost, dodatek polivinil alkohola pa poveča velikost delcev (3 mm) in zniža njihovo polidisperznost.

motion of PM chains increases with functional groups concentration and above the concentration of 0.25 mmol g^{-1} PM segments assess faster motion suggesting a change in the local packing density and domain structure.

- Polyaniline (PANI) and the copolymers of 2- and 3-substituted anilines were doped by 1M HCl, larger protonic acids (oxalic acid, p-toluensulfonic acid, 5-sulfosalicilic acid, HClO4) and a polymeric dopant - polyacrylic acid. The films of doped substituted polyanilines exhibited somewhat worse mechanical properties, but higher conductivity than dedoped PANI.
- We continued with the development of ionic conducting polymer membranes (cooperation with L13) on the basis of a fluorinated polymer filled with organo - inorganic fillers. In the last phase of the project we optimized the composition and established the correlation between composition and ionic conductivity. Basic preparation methods for one and multiple - layered membranes were investigated as well.
- We started the investigation on polymer-based nanocomposites using modified montmorillonite (MMT). MMT is a layered alumosilicate with weakly bound Na or Ca ions. The polarity of the MMT surface layer can be changed with quaternary ammonium salts thus enabling the preparation of polymer nanocomposites. The MMT modified by liquid crystalline quaternary ammonium salts were used for *in situ* solution polymerisation of liquid crystalline intercalated polyester nanocomposites.
- Copper (I) oxide and metallic copper particles were prepared by the polyol method from Cu acetate and Cu acetylacetonate (cooperation with L02). The reduction of Cu compounds to metal copper in di(ethylene glycol) takes place above 195 °C whereas in 1,2-propane above 175 °C. The particle size is of order 100 nm and increases with the in-

- Nadaljevali smo z raziskavo biorazgradljivih kopolimerov na osnovi asparaginske in mlečne kisline ali laktida. Podrobno smo raziskali sposobnost sintetiziranih kopolimerov za vezavo cinkovih ionov, ki je ključna za predvideno uporabo kopolimerov za nosilce zdravilnih učinkovin. V sodelovanju z L12 smo razvili novo metodo za določanje koncentracije cinka s fluorescenčno spektroskopijo. Vezava cinka je odvisna od vsebnosti aspartatnih enot v kopolimeru.
- Znanje s področja degradacije polimerov smo v sodelovanju s strokovnjaki Biotehniške fakultete Univerze v Ljubljani prenesli na razgradnjo lesa in pripravili utekočinjeni les. Pri tem smo razvili metodo utekočinjanja z sočasno sintezo poliestrov, kjer kot regente uporabljamo glikole in anhidride organskih kislin. Za utekočinjanje smo uporabili tudi mikrovalove, kar je omogočilo hitrejšo rekcijo. Ugotovitve so bile zaščitene s tremi slovenskimi patentnimi prijavami.
- V letu 2004 smo pričeli z raziskavami uporabe odpadnega polietilentereftalata (PET) za proizvodnjo smol in premazov. Postopek temelji na glikolizi PET in nadaljnjem zaestrenju dobljenih poliolov v nasičene ali nenasičene poliestre. Nenasičeni poliestri so že končni produkti, medtem ko so nasičeni poliestri surovina (poliol) za pripravo poliuretanov.
- V sodelovanju z L01 in FKKT UL smo raziskali vpliv temperature in časa staranja na reorganizacijo strukture ter termične in reološke lastnosti komercialnih visoko razvejenih alifatskih poliestrov (Boltorn HX, Perstorp). Do urejanja strukture med staranjem pride zaradi številnih linearnih sekvenc in nastajanja vodikovih vezi med hidroksilnimi in karbonilnimi ali drugimi hidroksilnimi skupinami. Najpomembnejša parametra, ki vplivata na termične in reološke lastnosti visoko razvejenih alifatskih poliestrov, sta stopnja razvejanja in molska masa.

creased concentration of the selected Cu compound. The addition of protective polymer colloids poly(vinyl pyrrolidone) and poly(methacrylic acid) reduces the agglomeration of Cu particles and their particle size, while the addition of poly(vinyl alcohol) increases the particle size (3 mm) and reduces their polidispersity.

- We continued investigating the biodegradable polymers based on aspartic and lactic acids or lactide. Capability of the copolymers for attachment of metal ions, which is crucial for their anticipated uses as carriers for controlled drug release, was explored in detail. A method was developed (cooperation with L12) to estimate the interactions between zinc ions and the copolymers by fluorescence spectroscopy.
- Knowledge on chemical degradation of polymers was extended to chemical degradation of wood and preparation of liquified wood. A method was developed of the combined liquefaction of wood and synthesis of polyesters using glycols and acid anhydrides as reagents. Wood was also liquified by using microwaves which accelerated the reaction significantly. The innovation was protected by three Slovenian patent applications.
- In 2004, we started the investigation on the application of waste polyethylene terephthalate (PET) for production of synthetic resins and coatings. Process is based on glycolysis of PET and subsequent esterification of the obtained polyols to saturated or unsaturated polyesters. Saturated polyesters are raw materials for polyurethane production whereas unsaturated polyesters are end-products.
- In cooperation with L01 and Faculty of Chemistry and Chemical Technology of the University of Ljubljana, Slovenia, we investigated the effects of annealing on the rearrangement of H-bonding structure and its influence on the thermal and rheological properties of commercial hyperbranched (HB) aliphatic

- V zadnji fazi evropskega projekta WHEYPOL smo dopolnili metodo za podrobno strukturno analizo polihidroksialkanoatnih kopolimerov ter terpolimerov z NMR visoke ločljivosti (600 MHz). Z analizo smo določili podrobno porazdelitev posameznih monomernih enot, kar je mogoče korelirati z lastnostmi polimerov. Za potrebe partnerjev v projektu smo opravljali SEC-MALS in NMR analize porazdelitve molskih mas in strukture.
- Izdelani so bili postopki za karakterizacijo praškastih in nehlapnih farmacevskih učinkovin ter pomožnih materialov z inverzno plinsko kromatografijo (IGC). Različnim celuloznim vlaknom, papirju in polivinilpirolidonu smo določili disperzijski del površinske energije, kislost oz. bazičnost po Lewisu, temperaturo steklastega prehoda in topnostne parametre.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Renault, Francija; protonsko prevodne visoko temperaturne membrane za gorivne celice (odg. nosilec iz L13)
- Razvojno tehnološki inštitut Savatech d.o.o., Kranj; sodelovanje pri raziskovalnem programu na področju elastomernih nanokompozitov
- Color d.d., Medvode; sodelovanje pri aplikativnem projektu na področju uporabe odpadnega polietilentereftalata
- Saturnus Embalaža d.d., Ljubljana; optimizacija proizvodnih procesov
- Za različne partnerje iz industrije (Kolektor d.o.o., Idrija; Plama-pur d.d., Podgrad; Termo d.d., Škofja Loka; Julon d.d., Ljubljana; Lek d.d., Ljubljana; Proizvodnja kemičnih izdelkov TKK Srpenica d.d., Srpenica; Elan Begunje;...) analiziramo polimerne materiale in rešujemo strokovne probleme

polyesters (Boltorn HX, Perstorp). Structure becomes more ordered as a consequence of numerous linear sequences and formation of multiple intermolecular H-bonds (–OH…O=C< and/or –OH…–OH). Crucial parameters affecting the thermal and rheological properties of HB polyesters are the degree of branching and molar mass.

- In the last phase of the European project Wheypol we complemented the methods for detailed structural characterization of hydroxyalkanoate copolymers using high resolution NMR (600 MHz). The distribution of comonomer units in the polymer chains was correlated to the polymer properties. The SEC-MALS and NMR analyses of various polyhydroxyalkanoates were performed for members of the project team.
- We developed methods for the characterization of powder and nonvolatile pharmaceutical and auxiliary materials using inverse gas chromatography (IGC). The dispersion part of the surface energy, Lewis basicity and acidity, the glass transition temperature, and solubility parameters of various cellulose fibres, paper and poly(vinyl pyrrolidone) were determined.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Renault, France; proton conductive high-temperature polymer membranes for fuel cells (principal investigator from L13)
- Research & Technology Institute Savatech d.d., Kranj, Slovenia; elastomer-based nanocomposites (programme)
- Color d.d., Medvode, Slovenia; the application of waste polyethylene terephthalate (applied project)
- Saturnus Embalaža d.d., Ljubljana, Slovenia; optimisation of production processes
- We analyse polymeric materials and solve professional problems for our industrial partners (Kolektor d.o.o., Idrija, Slovenia; Plama-

MEDNARODNO SODELOVANJE

- Projekt, 5. OP EU, 2002 - 2004: Dairy industry waste as source for sustainable polymeric material production, WHEYPOL
- Sodelovanje pri projektu 5. OP EU, 2001 - 2004: Advanced PEM fuel cells, APOLLON (odg. nosilec iz L13)
- Mreža odličnosti, 6. OP EU, 2004 - 2008: Nanostructured and functional polymer - based materials and nanocomposites, NANOFUN-POLY
- Slovensko - hrvaški bilateralni projekt, 2003 - 2004 (Institut Ruđer Bošković, Zagreb, Hrvaška): Struktura in dinamika prepletenih polimernih mrež
- Slovensko - italijanski bilateralni projekt, 2003 - 2005 (University of Pisa, Italija, Department of Chemistry and Industrial Chemistry): Okoljsko razgradljivi polimerni materiali in plastika v Sloveniji
- Bilateralni projekt Slovenija - Srbija in Črna gora, 2004 - 2005 (Tehnološko metalurški fakultet, Univerza v Beogradu, Srbija in Črna gora): Biorazgradljivi polimeri

POMEMBNI INŠTRUMENTI IN OPREMA

- Diferenčni dinamični kalorimeter Pyris 1, Perkin Elmer
- FTIR spektrometer 1725X, Perkin Elmer
- Plinski kromatograf GC 8700, Perkin Elmer
- Souporaba plinskega kromatografa Hewlett Packard Agilent 6890N z masno selektivnim detektorjem 5973N
- Tekočinski kromatograf z UV, RI (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
- Souporaba mikrovalovne pečice Milestone MLS 1200 Mega

pur d.d., Podgrad, Slovenia; Termo d.d., Škofja Loka, Slovenia; Julon d.d., Ljubljana, Slovenia; Lek d.d., Ljubljana, Slovenia; TKK Srpenica d.d., Srpenica, Slovenia, Elan, Slovenia; ...)

INTERNATIONAL COLLABORATION

- 5. OP EU, 2002 - 2004: Dairy industry waste as source for sustainable polymeric material production, WHEYPOL
- Collaboration within 5. OP EU, 2001 - 2004: Advanced PEM fuel cells, APOLLON (principal investigator from L13)
- Network of Excellence, 6. OP EU, 2004 - 2008: Nanostructured and functional polymer -based materials and nanocomposites, NANOFUN-POLY
- Bilateral Slovenian - Croatian project: 2003 - 2004 (Institut Ruđer Bošković, Zagreb, Croatia): Structure and dinamics of interpenetrating polymer networks
- Bilateral Slovenian - Italian project, 2003 - 2005 (University of Pisa, Italy, Department of Chemistry and Industrial Chemistry): Environmentally degradable polymeric materials and plastics in Slovenia
- Bilateral project Slovenia - Serbia and Montenegro, 2004 - 2005 (University of Belgrade, Serbia and Montenegro): Biodegradable polymers

MAJOR EQUIPMENT

- Differential scanning calorimeter Pyris 1, Perkin Elmer
- FTIR spectrometer 1725X, Perkin Elmer
- Gas chromatographs GC 8700 and Sigma 3, 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), and ELS 2100 detectors (Polymer Laboratories) for SEC measurements and for two-dimensional chromatography

- Souporaba velike inštitutske opreme (NMR, XRD, LC-MS, SEM)
- 60-l polindustrijski reaktor Bianchi

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Mag. Jelena Čulin z Instituta Ruđer Bošković, Zagreb, Hrvaška, je zagovarjala doktorsko disertacijo na Univerzi v Zagrebu. Delo na delno prepletenih polimernih mrežah je bilo opravljeno v sodelovanju z L07
- Nataša Filipič (diplomsko delo VSŠ, delovni mentor Miroslav Huskić)
- Dr. Gabriela Ambrožič je februarja 2004 zaključila enoletni raziskovalni obisk pri prof. Mauriziu Pratu na Fakulteti za farmacijo Univerze v Trstu, Italija
- Dr. Jelena Čulin, Institut Ruđer Bošković, Zagreb, Hrvaška; enotedenski raziskovalni obisk (bilateralni projekt)
- Dragana Pepić, doktorandka Univerze v Beogradu, Srbija in Črna Gora; dvotedenski raziskovalni obisk (bilateralni projekt)
- Jan Svoboda, doktorand Karlove Univerze iz Prage, Češka; enotedenski raziskovalni obisk

EVROPSKA MREŽA ODLIČNOSTI NANOFUN-POLY

Uraden začetek aktivnosti evropske mreže odličnosti v 6. okvirnem programu z naslovom Nanostructured and Functional Polymer-Based Materials and Nanocomposites, akronim Nanofun-poly, v kateri sodeluje Kemijski inštitut, je 1. 6. 2004. Mreža združuje 29 partnerjev, od tega je 12 tim. »core« partnerjev, ki so odgovorni za integracijo, koordinacijo in vodenje raznovrstnih aktivnosti mreže, medtem ko 17 pridruženih («satellite«) partnerjev sodeluje pri raziskovalnih aktivnostih in širjenju odličnosti. Koordinator je italijanski Konzorcij za znanost in tehnologijo materialov, konzorcij italijanskih univerz; koordinator mreže pa je prof. dr. Jose M. Kenny, Univerza v Perugi, Italija. Člani mreže prihajajo iz skupno 19 držav, od

- Liquid chromatograph with a multi-angle light scattering photometer Dawn DSP (Hewlett Packard, Wyatt Technology Corporation) for SEC-MALS measurements
- Joint use of a microwave oven Milestone MLS 1200 Mega
- Joint use of large Institute's equipment (NMR, WAXS, LC-MS, SEM)
- 60-l pilot reactor Bianchi

EDUCATION AND IMPORTANT VISITS

- Jelena Čulin, M.Sc., defended her Ph.D. thesis at the University of Zagreb, Croatia. The work on semi-interpenetrated polymer networks was performed in collaboration with L07.
- Nataša Filipič, diploma work, working mentor: Miroslav Huskić.
- Dr. Gabriela Ambrožič was one year visiting researcher with Prof. Maurizio Prato at the Faculty of Pharmacy, University of Trieste, Italy.
- Dr. Jelena Čulin, Institut Ruđer Bošković, Zagreb; one - week research visit (bilateral project).
- Dragana Pepić, Ph.D. student of the University of Belgrade, Serbia and Montenegro; two -week research visit (bilateral project).
- Jan Svoboda, Ph.D. student of the Charles University, Prague, Czech Republic; one - week research visit.

EUROPEAN NETWORK OF EXCELLENCE NANOFUN-POLY

June 1, 2004, is the official start of the European Network of Excellence (NoE, 6th Framework Programme) entitled Nanostructured and Functional Polymer-Based Materials and Nanocomposites, acronym Nanofun-poly, with the participation of the National Institute of Chemistry. The Nanofun-poly Consortium consists of 29 partners, 12 core partners and 17 satellite partners. Core partners have the responsibility of integration and coordinate and

teh jih je 14 iz Evrope, ostali pa so iz Argentine, Izraela, Kitajske, Turčije in ZDA. V industrijskem svetu mreže sodeluje okoli 30 malih, srednje velikih in velikih podjetij, podporo pa je izrazilo več kot 70 podjetij, organizacij, ministrstev in društev. Iz Slovenije so ustanovitev mreže podprli Lek Pharmaceuticals d.d., Ljubljana; Savatech d.d., Kranj; Grozd Plasttehnika, Ministrstvo za šolstvo, znanost in šport in Slovensko kemijsko društvo.

Glavni cilj Nanofun-poly je vzpostaviti mrežo odličnosti, ki naj bi postala evropska referenčna točka za nanostrukturne polimere in nanokompozitne materiale na osnovi polimerov, s tem da okrepi znanstveno in tehnološko odličnost ter odličnost šolanja in usposabljanja do- in podiplomskih študentov v vseh disciplinah, ki prispevajo k razvoju tega pomembnega področja. Multifunkcionalni nanostrukturni polimeri in polimerni nanokompoziti so pravzaprav ključni materiali za razvoj novih naprednih naprav. Aplikacije na osnovi novega znanja in naprednih tehnologij bodo pomembne za strateške industrijske veje, kot so npr. optoelektronika, telekomunikacije, embalaža, poljedeljstvo, gradbeništvo, avtomobilsko in letalsko industrijo, itd.

Zastavljeni cilj bo dosežen s sinergijo mednarodne odličnosti preko 100 raziskovalcev z različnih znanstvenih področij in multidisciplinarnega pristopa. Po formuli JPA (joint programme of activities) = JPI + JPR + JPS so naloge mreže: (a) integracija raziskovalnih zmogljivosti (JPI, joint programme of integration), (b) skupni raziskovalni program (JPR, joint programme of research), ki naj poveže posamezne institucije pri izvajanju skupnih projektov in (c) skupni program razširjanja odličnosti (JPS, joint programme of spreading of exellence). Končni cilj mreže je ustanovitev trajne integrirane organizacije raziskovalcev iz Evrope v povezavi z raziskovalci po svetu, ki bo usposobljena za raziskave, šolanje in prenos tehnologij na področju nanostrukturnih polimerov in polimernih nanokompozitov.

Kemijski inštitut se je v Nanofun-poly vključil s

manage the different NoE activities while satellite partners have access and participate in research and spreading activities. The coordinator is Consortium for Materials Science and Technology (INSTM), the Consortium of Italian Universities, while the Network coordinator is Prof. José M. Kenny of the University of Perugia, Italy. Partners come from 19 countries, 14 European ones, and from Argentina, China, Israel, Turkey and USA. The Industrial Council of the NoE consists of about 30 small, medium - sized and large enterprises while over 70 enterprises, organisations, ministries and professional associations gave their support to the Nanofun-poly, among them also Lek Pharmaceuticals d.d., Ljubljana, Slovenia; Savatech d.d., Kranj, Slovenia; Slovenian Plasttechnics Cluster; Ministry of Education, Science and Sport of the Republic of Slovenia and Slovenian Chemical Society.

The main objective of Nanofun-poly is to generate a Network of Excellence designed to become the European reference point on nanostructured polymers and polymer-based nanocomposite materials, strengthening the scientific, technological and training excellence in all the disciplines that contribute to the development of this important field. Multifunctional nanostructured polymers and polymer-based nanocomposites are, in fact, a key issue for the advanced development of new devices. Applications that will benefit from Nanofun-poly concern strategic industrial sectors such as optoelectronics, telecommunications, packaging, agriculture, building construction, automotive and aerospace, etc.

This objective will be reached through the synergy of international excellence of over 100 scientists of different scientific areas, and multidisciplinary approaches. According to equation JPA (joint programme of activities) = JPI (joint programme of integration) + JPR (joint programme of research) + JPS (joint programme of spreading of exellence), the objectives of Nanofun-poly are the following: (a) integration of research capacities to generate and

posameznimi raziskovalnimi dejavnostmi, aktivnosti pa koordinira L07 oz. doc. dr. Majda Žigon. Področja sodelovanja so: (a) sinteza in karakterizacija visoko razvejenih polimernih struktur (analiza strukture in porazdelitve molskih mas), (b) formiranje nanostruktur s nekovalentnimi in ionskimi interakcijami (raziskava mikro agregacije in nastajanja inkluzijskih teles nekaterih proteinov), (c) tehnike kontrolirane polikondenzacije in poliadicije vključno s sol-gel tehnikami, (d) funkcionalni nanodelci in priprava hibridnih struktur (modifikacija nanopolnil, sinteza kovinskih delcev, čistih ali mešanih oksidov), (e) nanostrukturni hibridni organsko - anorganski sistemi, formulacije z uporabo hibridnih struktur (priprava polimernih in elastomernih nanokompozitov z in-situ polimerizacijo ali z mešanjem v laboratorijskem dvopolžnem ekstruderju), (f) zamreženi sistemi (delno prepletene polimerne mreže).

Prvo srečanje in spoznavanje partnerjev mreže je potekalo 11. in 12. 10. 2004 v Lyonu, Francija, prva delavnica za polja odličnosti »polimerna kemija« in »predelava polimerov« pa je bila 27. - 29. 1. 2005 v Dresdnu, Nemčija. Sledi cela vrsta delavnic, šol, seminarjev in konferenc. Več o Nanofun-poly in o prireditvah, ki so odprte tudi za širši krog udeležencev, si lahko ogledate na spletni strani //www. nanofun-poly.com/.

install the new organisation, (b) jointly executed research to support the network's goals, and (c) activities designed to spread excellence. The final objective of NoE is to create a lasting integrated organisation of researchers at a European level, well connected with the rest of the world and able to lead research, education and technology transfer in nanostructured polymers and their nanocomposites.

The National Institute of Chemistry participates in the Nanofun-poly through individual research activities, coordinated by L07 and Assist. Prof. Majda Žigon. The fields of cooperation are the following: (a) Synthesis and characterization of hyperbranched polymer structures (full structural and molar mass analysis), (b) Nanostructure formation by self-assembly and ionic interactions (investigation of micro - aggregation and inclusion body formation of some properly folded proteins), (c) Controlled polycondensation and polyaddition techniques including sol-gel, (d) Functional nanoparticles and hybrid structure preparation (modification of nanofillers, synthesis of metallic particles, pure or mixed oxide particles), (e) Nanostructured hybrid organic-inorganic systems, formulations using hybrid structures (preparation of polymeric and elastomeric nanocomposites by in-situ polymerization or mixing the components using a twin screw extruder), (f) Crosslinked systems (semi - interpenetrating polymer networks).

The first meeting of the NoE partners took place on October 11 and 12, 2004, in Lyon, France and the frst Workshop on the areas of excellence Polymer Chemistry and Polymer Processing was on January 28 and 29, 2004, in Dresden, Germany. Many other spreading activities - workshops, training courses, seminars and conferences, open also to participants outside the NoE - will follow. More about Nanofun-poly and its activities can be seen at the Web page //www. nanofun-poly.com/.

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 (1/2)
Dr. Anton Štimac (do / until 30. 6. 2004)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Damjan Šterk

Laboratorij za organsko sintezo in kemijo zdravil
Laboratory for Organic and Medicinal Chemistry

PODROČJA DEJAVNOSTI

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

BIBLIOGRAFIJA

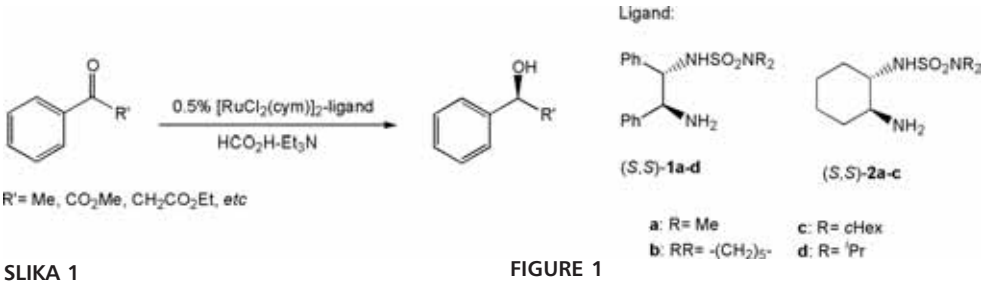
5 izvirnih znanstvenih člankov
1 objavljeni povzetek znanstvenega prispevka na konferenci
2 patentni prijavi
1 patent
1 predavanje na tuji univerzi
1 diploma
1 uredništvo revije

GLAVNI DOSEŽKI V LETU 2004

- Priprava nove serije kiralnih fosfinskih ligandov in njihovih kompleksov, ki kažejo visoko selektivnost in aktivnost pri asimetričnem hidrogeniranju funkcionaliziranih olefinov
- Razvoj novih substratov za aren-olefin tvorbo vezi (Heck reakcija)
- Razvoj praktičnih in ekonomičnih sintetskih poti do dveh farmacevtskih spojin

Asimetrično transfer hidrogeniranje

Iskanje ekonomičnih poti za pripravo enantiomerno čistih alkoholov v industrijskem merilu je neprestano aktualno zaradi njihove uporabe v sintezi farmacevtskih in agroživilskih učinkovin. Zelo atraktivna pot do enantiomerno čistih alkoholov je katalitska redukcija ketonov. Še



SLIKA 1

Asimetrično transfer hidrogeniranje različnih vrst ketonov

RESEARCH ACTIVITIES

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

BIBLIOGRAPHY

5 Original Scientific Articles
1 Published Scientific Conference Contribution Abstract
2 Patent Applications
1 Patent
1 Invited Lecture at a Foreign University
1 Undergraduate Thesis
1 Editorship

IMPORTANT ACHIEVEMENTS IN 2004

- Preparation of a new series of chiral phosphine ligands and their complexes which showed high selectivity and activity in asymmetric hydrogenation of functionalized olefines
- Development of novel substrates for arene-olefine coupling (Heck reaction)
- Development of practical and economical synthetic routes to two interesting pharmaceuticals

FIGURE 1

Asymmetric transfer hydrogenation of various classes of ketones

posebaj enostaven proces je transfer hidrogeniranje s propan-2-olom ali HCO_2H-Et_3N azeotropom, pri katerem se izognemo uporabi vodika pod visokim pritiskom ali drugih nevarnih reducentov.

Med opaznejšimi dosežki redukcije aromatskih ketonov je Noyorijev (Nobelov nagrajenec za kemijo 2001) kiralen Ru(II)-N-tozil-1,2-difeniletilendiaminski katalizator (Ru(II)-TsDPEN), ki kaže v nekaterih primerih visoko enantioselektivnost.

Zanimala nas je optimizacija Ru(II)-TsDPEN katalizatorja za redukcijo različnih vrst ketonov in odločili smo se modificirati sulfonamidni del liganda, pri čemer bi ostal NH_2 konec nespremenjen. Znano je namreč, da Ru(II)-TsDPEN na polimernem nosilcu (Beyston et al.) in Ru(II)-N-perfluorosulfonil-DPEN (Mioskowski et al.) kažeta v nekaterih primerih višje enantioselektivnosti.

Za namen hidrogeniranja s prenosom vodika so pripravili različne RSO_2-DPEN ligande z R= Ar, CF_3, R_F, ligandi z N-(dialkilamino)sulfamoilno skupino (R'_2N) pa so bili nezani.

Pripravili smo dve seriji novih *N*-(dialkilamino)sulfamoil-1,2-diaminskih ligandov 1a-d in 2a-c pri čemer smo izhajali iz DPEN ali iz trans-1,2-diaminocikloheksana (CYDA), in jih uporabili pri Ru(II) in Rh(III)-kataliziranem asimetričnem transfer hidrogeniranju različnih modelnih aromatskih ketonov do kiralnih alkoholov.

Z *in situ* pripravljenimi Ru(II) kompleksi teh ligandov smo dosegli dobro aktivnost v transfer hidrogeniranju pri 25°C z uporabo HCO_2H-Et_3N azeotropa. Enantioselektivnost in konverzija sta bila boljša v močno polarnih topilih kot so DMF, DMA, NMP, 1,3-dimetil-2-imidazolidinon, TMU, v primerjavi s MeCN, CH_2Cl_2 in toluenom. Povišanje temperature od sobne do 50°C je pospešilo redukcijo, vendar je bila enantioselektivnost manjša, medtem ko je bil pri 0°C reakcijski čas daljši in enantioselektivnost višja za 1-2%.

N-(Dimetilamino)sulfamoil-1,2-difeniletilendiamin ligand (1a) je bil v primerjavi z Noyorijevim TsDPEN-om še posebaj učinkovit,

Asymmetric transfer hydrogenation

The search for economic industrial routes towards the preparation of enantiomerically pure alcohols still continues owing to their use in pharmaceuticals and agrochemicals. A direct access to single enantiomer alcohols via catalytic reduction of ketones appears to be the most attractive. Transfer hydrogenation with propan-2-ol or HCO_2H-Et_3N azeotrope is a very convenient process eliminating high hydrogen pressure or hazardous reducing reagents. Amongst some notable achievements for the reduction of aromatic ketones, Noyori (2001 chemistry Nobel prize winner) chiral Ru(II)-N-tosyl-1,2-diphenylethylenediamine catalyst (Ru(II)-TsDPEN) displays high enantioselectivity. We were interested to optimize the Ru(II)-TsDPEN system for the reduction of various classes of ketones, and we thought to modify the sulfonamide residue maintaining the NH_2 terminus unchanged. As a matter of fact, the polystyrene supported Ru(II)-TsDPEN of Beyston et al. and the Ru(II)-N-perfluorosulfonyl-DPEN of Mioskowski et al. showed in some cases higher enantioselectivities.

Various RSO_2-DPEN ligands for transfer hydrogenation were already prepared with R= Ar, CF_3, R_F, but ligands with *N*-(dialkylamino)sulfamoyl group (R'_2N) were unknown.

We prepared two series of new *N*-(dialkylamino) sulfamoyl-1,2-diamine ligands derived either from DPEN 1a-d or from trans-1,2-diaminocyclohexane (CYDA) 2a-c and used them in Ru(II) and Rh(III)-catalyzed asymmetric transfer hydrogenation of various models of aromatic ketones leading to chiral alcohols.

The Ru(II) complexes of the above ligands were prepared and showed good activity in transfer hydrogenation at 25°C using HCO_2H-Et_3N azeotrope. Enantioselectivity and conversion were better in highly polar solvents such as DMF, DMA, NMP, 1,3-dimethyl-2-imidazolidinone, TMU compared to MeCN, CH_2Cl_2 and toluene. Increasing the temperature from r.t. to 50°C accelerated the reduction but gave lower enantioselectivity, while at 0°C prolonged re-

SLIKA 2
Sistem za hidrogeniranje

FIGURE 2
System for hydrogenation

saj je bil v nekaterih primerih bolj enantioselektiven. Pri redukciji etil benzoilacetata je vodil do 98% ee in 100% konverzije in z 2-karbometoksi-1-indanonom do anti-produkta (>99% de) z >99% ee in 87% konverzijo.
Ligand 1c je dal 85% ee in 100% konverzijo pri redukciji metilbenzoilformata. V primeru acetofenona je redukcija z različnimi ligandi rezultirala v do 96% ee in 80% konverziji.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Lek farmacevtska družba d.d., Ljubljana; Sinteza potencialnih farmacevtskih učinkovin
- Krka tovarna zdravil d.d., Novo mesto; Razvoj sinteze izbrane farmacevtske učinkovine
- Pliva - Research Institute, Zagreb, Hrvaška; Razvoj ključne stopnje v sintezi generične farmacevtske učinkovine
- PhosPhoenix SARL, Pariz, Francija; Razvoj novih industrijskih procesov na osnovi homogene katalize

POMEMBNI INŠTRUMENTI IN OPREMA

- HPLC in GC sistemi opremljeni s kiralnimi kolonami
- Polarimeter
- Ultra kriomat (-100 do +100 °C)

action time was required and resulted in 1-2% higher ee.
In particular, *N*-(dimethylamino)sulfamoyl-1,2-diphenylethylenediamine (1a) was an effective ligand compared to Noyori Ts-DPEN displaying a better enantioselectivity in some cases. In the reduction of ethyl benzoylacetate, it led to 98% ee and 100% conversion, and with 2-carbomethoxy-1-indanone it led to the anti-product (>99% de) in >99% ee and 87% conversion. Ligand 1c gave up to 85% ee and 100% conversion for the reduction of methylbenzoylformate. In the case of acetophenone, the reduction with the various ligands resulted in up to 96% ee and 80% conversion.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Lek Pharmaceuticals, d.d., Ljubljana, Slovenia; Synthesis of potential pharmaceutical compounds
- Krka d.d., Novo mesto, Slovenia; Development of new synthetic route for the preparation of a pharmaceutical compound
- Pliva - Research Institute, Zagreb, Croatia; Development of a key step to generic pharmaceutical
- PhosPhoenix SARL, Paris, France; Development of industrial processes based on homogeneous catalysis

MAJOR EQUIPMENT

- HPLC and GC systems equipped with chiral columns
- Polarimeter
- Ultra kryomat (-100 to +100 °C)

L09

Laboratorij za anorgansko kemijo in tehnologijo

Laboratory for Inorganic Chemistry and Technology

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Dr. Nataša Novak Tušar
Dr. Gregor Mali
Dr. Maja Mrak

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Mag. Alenka Ristić

PODIPLOMSKA ŠTUDENTA / GRADUATE STUDENTS
Matjaž Mazaj
Saša Vertelj

TEHNIČNO OSEBJE / TECHNICAL STAFF
Olga Gorše
Edi Kranjc
Mojca Opresnik

PODROČJA DEJAVNOSTI

Porozni materiali:
- zeolitni materiali
- mezoporozni materiali
- cement

Strukturna analiza:
- rentgenska difrakcija
- nuklearna magnetno resonančna spektroskopija
- rentgenska absorpcijska spektroskopija

http://www.ki.si/lab/l09/index.html

BIBLIOGRAFIJA

7 izvirnih znanstvenih člankov
2 objavljena znanstvena prispevka na konferencah (vabljeno predavanje)
3 objavljeni znanstveni prispevki na konferencah

RESEARCH ACIVITIES

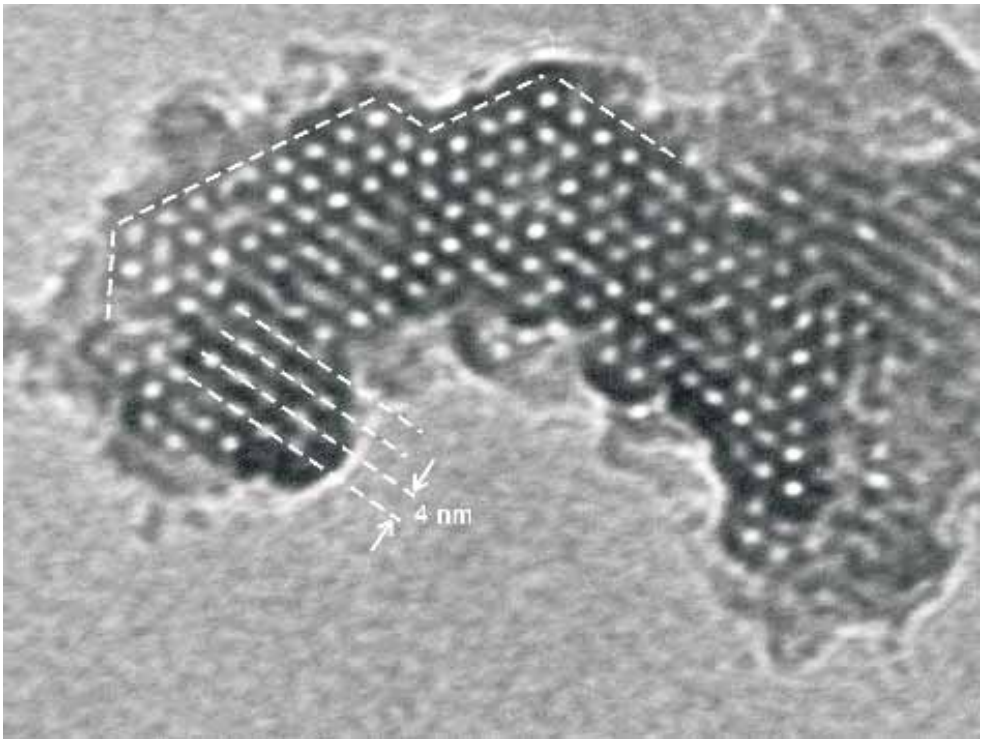
Porous materials:
- zeolitic materials
- mesoporous materials
- cement research

Structural research:
- X-ray diffraction
- NMR spectroscopy
- X-ray absorption spectroscopy

http://www.ki.si/lab/l09/index.html

BIBLIOGRAPHY

7 Original Scientific Articles
2 Published Scientific Conference Contributions (Invited Lecture)
3 Published Scientific Conference Contributions



SLIKA

Posnetek mezoporoznega silikata z elektronsko mikroskopijo z visoko ločljivostjo

FIGURE

HRTEM (High Resolution Transmission Electron Microscopy) image of mesoporous silicate

10 objavljenih povzetkov znanstvenih prispevkov na konferencah
2 predavanji na tujih univerzah
1 vabljeno predavanje na konferenci brez natisa
1 doktorat
3 uredništva revij

10 Published Scientific Conference Contribution Abstracts
2 Invited Lectures at Foreign Universities
1 Unpublished Invited Lecture at a Conference
1 Doctoral Dissertation
3 Editorships

GLAVNI DOSEŽKI V LETU 2004

Zeolitni materiali

- Sintetizirali smo z železom funkcionaliziran aluminofosfat VPI-5, ki ga bomo uporabljali kot katalizator pri oksidaciji linearnih alkenov. Z nizom spektroskopskih metod (XANES, EXAFS in IR spektroskopija) smo analizirali katalitsko aktivna mesta v sintetiziranem materialu. V FeVPI-5 je železo prisotno v obliki Fe(III). Kljub oktaedrični koordinaciji Fe(III) ionov smo dokazali, da smo železo vgradili v ogrodje aluminofosfata, ki ima zato dobre katalitske lastnosti. To potrjuje tudi spremljanje adsorpcije in desorpcije CO na oksidiran in reduciran material z IR spektroskopijo, ki kaže na prisotnost kislih ter redoks mest v FeVPI-5.
- Študirali smo vlogo strukturnega usmerjevalca 1,2-diaminopropana (DAP) pri hidrotermalni sintezi železovega(III) fosfata (FAPO-DAP). FAPO-DAP nastane pri 180°C v enem dnevu. Daljši kristalizacijski časi vodijo do nastanka mešanice FePO-DAP in leukofosfita. Izračuni mrežnih in prostih energij dokazujejo razpad strukturnega usmerjevalca že pred nastankom leukofosfita.
- Raziskovali smo kinetiko hidrotermalne kristalizacije ortorombske modifikacije karnegita iz amorfnega aluminosilikata. Ugotovili smo, da karnegit kristalizira s homogeno nukleacijo v difuzijsko kontroliranem procesu enodimenzionalne rasti kristala. Posledica enodimenzionalne rasti kristala je nastanek igličastih kristalov karnegita.
- Sodelovanje s podjetjem Silkem d.o.o., Kidričevo na projektu z naslovom »Razvoj

IMPORTANT ACHIEVEMENTS IN 2004

Zeolitic materials

- Iron - functionalised aluminophosphate VPI-5 was synthesised as catalyst for oxidation reaction of linear alkenes. Catalytically active sites were studied by a set of spectroscopic techniques (XANES, EXAFS and IR) in prepared material. It was shown that Fe(III) ions were present in FeVPI-5. Although they occupy octahedral positions, they are incorporated into aluminophosphate framework, thus generating catalytically active sites. The latter property is confirmed also by monitoring IR spectra during the adsorption and desorption of CO on an oxidized and reduced FeVPI-5, which show the presence of acid and redox sites in the material.
- The structure - directing role of 1,2-diaminopropane (DAP) in the hydrothermal synthesis of iron(III) phosphate (FAPO-DAP) was studied. FAPO-DAP was formed at 180 °C in one day. Longer crystallization yielded a mixture of FePO-DAP and leucophosphite. Lattice energy and free energy calculations strongly supported the supposition that a decomposition of DAP occurred prior to the formation of leucophosphite.
- Kinetics of the hydrothermal crystallization of orthorhombic modification of low-carnegieite from precipitated amorphous aluminosilicate was investigated. Kinetic analyses have shown that the crystallization of low- carnegieite occurs by homogeneous nucleation of low - carnegieite inside the matrix of amorphous aluminosilicate precursor and diffusion -controlled one - dimensional growth of the nuclei. The consequence of the one-dimensional crystal growth is the

tehnologije kompaktiranja zeolita« smo zaključili z uvedbo nove tehnologije kompaktiranja praškastih zeolitov. Takšna tehnologija omogoča kontinuirno proizvodnjo granulata z nasipno težo do 800 g/L ter z velikostjo kompaktiranih zrn do 3 mm. Produkti so brezprašne komponente kompaktnih pralnih praškov, z znatno izboljšanimi fizikalno - kemijskimi in pralnimi lastnostmi.

Mezoporozni materiali

- Sintetizirali smo različne s titanom funkcionalizirane silikatne porozne materiale, ki smo jih testirali kot katalizatorje v epoksidaciji ciklooktena: mikroporozen Ti-BETA, mezoporozen Ti-MCM-41 in mikro / mezoporozen kompozit Ti-BETA/MCM-41. Reakcija epoksidacije ciklooktena s *tert*-butil hydroperoksidom (*t*-BHP) kot oksidantom je imela najboljši izkoristek z mezoporoznim Ti-MCM-41.

Cement

- V raziskavah za Salonit Anhovo d.d., Deskle smo ugotavljali vpliv mineralnih dodatkov (različnih tipov karbonatov) na fizikalno - kemijske lastnosti hidravličnega sistema portlandski cement - mineralni dodatek.
- Podrobna študija poznavanja vpliva karbonatnih ionov na razvoj hidratiziranih faz v sistemu portlandski cement - mineralni dodatek nam je omogočila bolj smiselno posredno izbiro lastnosti hidravličnega sistema glede na zahteve predvidenih aplikacij.

Strukturna analiza

- Z metodo rentgenske difrakcije na monokristalih smo analizirali in določili strukturi dveh organokovinskih spojin, kjer so cinkovi atomi premreženi z organskimi tereftalatnimi skupinami v tridimenzionalno oziroma verižno strukturo. Poteg tega smo določili novi anorgansko - organski strukturi,

formation of the needle - shaped crystals of low - carnegieite.

- The cooperation with Silkem d.o.o., Kidričevo, Slovenia on the project entitled »The Development of Technology for the Compaction of Zeolite« resulted in the introduction of a new technology of zeolite compaction that enabled the continuous production of granulate having bulk density of up tp 800 g/L and with an average diameter of granules of up to 3 mm. This product represents a non - dusting variety of compacted washing powders (compounds) and possesses significantly improved physico - chemical and health - related properties.

Mesoporous materials

- Different titanium - functionalised porous silicates (microporous Ti-BETA, mesoporous Ti-MCM-41 and micro/mesoporous composite Ti-BETA/MCM-41) were synthesized and tested as catalysts in oxidation reactions. In the epoxidation of cyclooctene using *tert*-butyl hydroperoxide (*t*-BHP) as the oxidant the best yield was obtained with mesoporous Ti-MCM-41 as catalyst.

Cement research

- The research with collaboration with Salonit Anhovo d.d., Deskle, Slovenia included studies on the effects of mineral admixtures (different carbonates) on the physico - chemical properties of the system portland cement - mineral admixture.
- The detailed knowledge of the influence of different carbonate admixtures on the development and nature of hydrated phases in the system portland cement - mineral admixture enabled the design of optimal formulations/ properties for specific applications.

Structure determination

- Single - crystal X-ray diffraction method was used for structure determination and analysis of two organo - metallic compounds, where zinc atoms were bonded to organic tetrphthalic groups and formed a three - di-

ki ju sestavljajo aluminofosfatne plasti premrežene z organskimi molekulami in kationi, ki sta bili pripravljeni, kot del študije poroznih anorgansko - organskih hibridnih struktur kot potencialnih adsorbentov (skladiščenje vodika).

- Z jedrsko magnetno resonanco smo študirali nekatere aluminofosfatne in aluminosilikatne mikro - in mezoporozne materiale. Pokazali smo, da s pomočjo spektrov fosforjevih jeder lahko nedvoumno potrdimo vgradnjo ionov Ni(II), Co(II), Fe(II/III) in Mn(III) v ogrodja aluminofosfatnih materialov in da z natančno analizo spektrov lahko določimo celo količino vgrajene prehodne kovine in opišemo njeno porazdelitev po vzorcu. Metoda zaznava hiperfino sklopitev med ioni prehodne kovine in jedri fosforja in je zato komplementarna mnogim drugim tehnikam (XAS, Mössbauerjeva spektroskopija), ki opazujejo le bližnjo okolico prehodne kovine. Komplementarna je tudi spektroskopiji ENDOR in ESEEM, saj za razliko od slednjih omogoča meritve na vzorcih, ki vsebujejo zmerne ali celo zelo velike količine paramagnetnih snovi.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Salonit Anhovo d.d., Deskle; raziskave in razvoj cementov z apnencem in mineralnimi dodatki
- Silkem d.o.o., Kidričevo; razvoj tehnologije kompaktiranja zeolita
- Lek d.d., Ljubljana; rentgenska praškovna analiza in določanje specifične površine
- Krka d.d., Novo mesto; rentgenska praškovna analiza in določanje specifične površine

MEDNARODNO SODELOVANJE

Gostujoči raziskovalci:

- Prof. Leiv K. Sydnes, (predsednik IUPAC), Univerza v Bergnu, Norveška
- Prof. David StC. Black, Univerza NSW, Sydney, Avstralija

mensional and a chain structure, respectively. Two new inorganic - organic structures with aluminophosphate layers and intercalated organic molecules were determined as a part of our studies of porous inorganic - organic hybrid structures as potential adsorbents (hydrogen storage).

- Solid state nuclear magnetic resonance was used to study several micro- and mesoporous aluminophosphate and aluminosilicate materials. Broadline phosphorus NMR spectroscopy provided direct evidence on incorporation of Ni(II), Co(II), Fe(II/III) and Mn(III) ions into aluminium framework sites of selected aluminophosphate molecular sieves. Quantitative analysis of NMR spectra yielded information about the distribution and about the amount of the incorporated transition metals within the bulk material. Because it detects interaction between transition metal ions and phosphorus nuclei, that is the interaction that extends beyond the first coordination shell, broadline phosphorus NMR spectroscopy is complementary to XAS and Mössbauer spectroscopy. It is also complementary to ESEEM and ENDOR spectroscopy, because it allows measurement of hyperfine coupling constants in metal phosphates and in MeAlPO materials with larger amounts of transition metals.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Salonit Anhovo d.d., Deskle, Slovenia; investigations and development of cements with limestone and mineral admixtures
- Silkem d.o.o., Kidričevo, Slovenia; development of technology for zeolite compacting
- Lek d.d., Ljubljana, Slovenia; X-ray powder diffraction analyses and determination of specific surface areas
- Krka d.d., Novo mesto, Slovenia; X-ray powder diffraction analyses and determination of specific surface areas

- Prof. Nevenka Rajić, Tehnološko - metalurška fakulteta, Univerza v Beogradu, Srbija in Črna gora
- Sanja Šajić, Tehnološko - metalurška fakulteta, Univerza v Beogradu, Srbija in Črna gora
- Mario Šiljeg, Fakultet kemijskog inženjerstva in tehnologije, Sveučilište Zagreb, Hrvaška
- Vedrana Grozdanić, Fakultet kemijskog inženjerstva in tehnologije, Sveučilište Zagreb, Hrvaška
- Mag. Karmen Margeta, Fakultet kemijskog inženjerstva in tehnologije, Sveučilište Zagreb, Hrvaška
- Prof. Antoine Gedeon, Univerza Pierre in Marie Curie, Pariz, Francija
- Dr. Frank Launay, Univerza Pierre in Marie Curie, Pariz, Francija
- Dr. Martin Attfield, UMIST, Manchester, Anglija

V mednarodnih projektih:

- Šesti okvirni program Evropske unije, NoE FP6 INSIDE_PORES (2004 - 2008), koordinator: National Center for Scientific Research "Demokritos", Atene, Grčija
- ESRR - Evropski sklad za regionalni razvoj, Center odličnosti "Nanoznanosti in nanotehnologije" (2004 - 2007)
- ESRR - Evropski sklad za regionalni razvoj, NMR center odličnosti za študij struktur in interakcij v biotehnologiji in farmaciji (2004 - 2007)
- Slovensko - francoski bilateralni projekt, PROTEUS (2003 - 2004), Univerza Pierre in Marie Curie, Pariz, Francija
- Slovensko - angleški bilateralni projekt, PARTNERSHIP IN SCIENCE (2003 - 2004), UMIST, Manchester, Anglija
- Slovensko - srbski bilateralni projekt (2004 - 2005), Tehnološko - metalurška fakulteta, Beograd, Srbija in Črna gora
- Projekt z Univerzo v Manchestru v okviru sporazuma o znanstvenem sodelovanju med

INTERNATIONAL COLLABORATION

- The 6th Framework Programme of the European Union, NoE FP6 INSIDE_PORES (2004 - 2008), Coordinator: National Center for Scientific Research "Demokritos", Athens, Greece
- ERDF - The European Regional Development Fund, Centre of excellence "Nanoscience and nanotechnology" (2004 - 2007)
- ERDF - The European Regional Development Fund, NMR Centre of excellence for the study of structures and interactions in biotechnology and pharmacy (2004 - 2007)
- Slovenia - France bilateral project, PROTEUS (2003 - 2004), University Pierre et Marie Curie, Paris, France
- Slovenia - UK bilateral project, PARTNERSHIP IN SCIENCE (2004 - 2005), UMIST, Manchester, UK
- Slovenia - Serbia bilateral project (2004 - 2005), Faculty of Technology and Metallurgy, University of Belgrade, Serbia and Montenegro
- Project with University of Manchester within the frame of an agreement for scientific cooperation between Slovenian Academy of Sciences and Arts (SAZU) and The Royal Society, London, Great Britain
- One - year Marie Curie Postdoctoral Fellowship (MCFI-2002-00811), University of Trieste and Sincrotron ELETTRA, Trieste, Italy (Nataša Novak Tušar)

MAJOR EQUIPMENT

- X-ray powder diffractometer Siemens D 5000 for measurements of powder patterns with high resolution at high temperatures from 50 to 1450°C, at low temperatures from boiling point of liquid nitrogen to 400°C in vacuum or other atmospheres and for measurements of thin films
- Tristar 3000, an automated gas adsorption analyser (Micromeritics Instrument Co.) for surface area (BET) measurements, adsorption

SAZU in The Royal Society, London, Velika Britanija

- Enoletna podoktorska Marie Curie štipendija (MCFI-2002-00811, 2003 - 2004) na Univerzi v Trstu in na sinhrotronu ELETTRA v Trstu, Italija (Nataša Novak Tušar)

POMEMBNI INŠTRUMENTI IN OPREMA

- Rentgenski praškovni difraktometer Siemens D 5000 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 in volumna, ter porazdelitve por praškastih vzorcev
- SDT 2960 sistem za termično analizo, DSC-TGA (TA Instruments Inc.) omogoča simultane meritve energijskega pretoka in masnih sprememb v materialih od sobne temperature do 1500°C
- Sistem za termično nalizo (model TA 2000, TA Instruments Inc.), ki je sestavljen iz TGA (1200°C) in DSC (725°C) modulov
- Microtrac S3500, aparatura za določevanje velikosti in porazdelitev delcev v mokrem ali suhem stanju. Območje meritev za mokre vzorce od 0.02 μm do 1400 μm in za suhe vzorce od 0.25 μm do 1400 μm
- Autopycnometer (Micromeritics Instrument Co.) aparatura za samodejno določevanje gostote materialov s helijem
- Centrifuga Hettich, Rotanta 460 R hlajena (temperaturno območje od –20°C do + 40°C). Hitrost obratov od 500 do 9.500 min^{-1}
- Ultra Turrax disperzer T25 (IKA)
- Mikrovalovna peč MLS-1200 MEGA (Milestone)
- Mikrovalovna peč ETHOS (Milestone)

isotherms and volume, area and pore distribution of powder samples (pore diameters from 300 nm to 1.7 nm using nitrogen)

- SDT 2960 system for thermal analysis, DSC-TGA (TA Instruments Inc.) for simultaneous measurements of enthalpy and mass changes in materials (from room temperature to 1500°C)
- System for thermal analysis (model TA 2000, TA Instruments Inc.), TGA (1200°C) and DSC (725°C) modules
- Microtrac S3500 Particle Size Analyzer, wet or dry samples. The range of measurement for wet samples is from 0.02 μm to 1400 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°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)

EDUCATION AND IMPORTANT VISITS

Education:

- Dr. Nataša Zabukovec Logar was elected assistant professor for the field of chemistry at Nova Gorica Polytechnic, Slovenia
- Dr. Andrej Horvat ended his Ph.D. on 1. 12. 2004; co - supervisor: Prof. Venčeslav Kaučič

Important visits:

- Prof. Leiv K. Sydnes, (President of IUPAC), University of Bergen, Norway
- Prof. David StC. Black, University NSW, Sydney, Australia
- Prof. Antoine Gedeon, University Pierre et Marie Curie, Paris, France

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

- Dr. Nataša Zabukovec Logar je bila 23. 9. 2004 izvoljena v naziv docent za področje kemije na Politehniki Nova Gorica
- Dr. Andrej Horvat je doktoriral 1. 12. 2004; komentor prof. Venčeslav Kaučič

L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry

VODJA / HEAD
Doc. dr. Janko Jamnik

RAZISKOVALCI / RESEARCHERS
Dr. Marjan Bele
Dr. Robert Dominko
Doc. dr. Miran Gaberšček

MLADI RAZISKOVALCI /
YOUNG RESEARCHERS
Boštjan Genorio
Dušan Strmčnik

TEHNIČNO OSEBJE / TECHNICAL STAFF
Milena Zorko

PODROČJA DEJAVNOSTI

Materiali za energijske in informacijske tehnologije

Podrobnejša opredelitev:

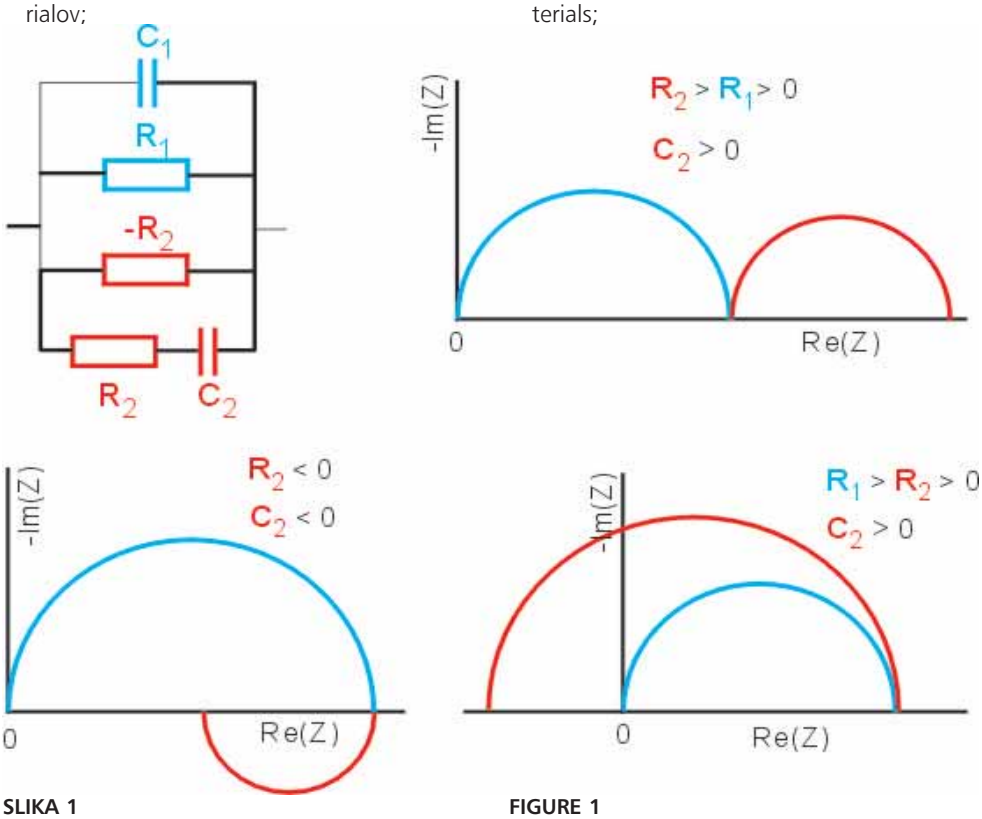
- študij kinetike transporta in sprememb kemijske sestave v trdnih mešanih prevodnikih; vpliv površin;
- vpliv nanostrukturiranosti trdnih kompozitov na izbrane lastnosti, kot so elektrokemijsko shranjevanje energije, raztapljanje, elektrokataliza ipd. (uporaba v energetiki, informatiki, farmaciji);
- priprava in karakterizacija nanometrskih ovojnic okoli funkcionalnih delcev;
- priprava nanometrskih filmov na zunanjih in / ali notranjih površinah funkcionalnih materialov;

RESEARCH ACTIVITIES

Materials for energy and information technologies

Detailed clasification:

- Study of transport kinetics and chemical composition changes in solid mixed conductors; influence of surfaces on these phenomena;
- 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;



SLIKA 1

Splošna nadomestna shema in impedančni spektri za primer enega tipa adsorbiranega intermediata/produkta pri poljubnem mehanizmu elektrokemijske reakcije na fazni meji kovina/elektrolit.

FIGURE 1

General equivalent circuit and corresponding impedance spectra for one adsorbed intermediate/product at the metal/electrolyte interface.

- vgradnja funkcionalnih materialov v ustrezne matrike;
- vpliv površinskega naboja na stabilnost disperzij ter suspenzij; polielektrolitske titracije.

BIBLIOGRAFIJA

7 izvirnih znanstvenih člankov
1 strokovni članek
1 poljudni članek
1 drugi članek in sestavek
1 objavljeni znanstveni prispevek na konferenci (vabljeno predavanje)
7 objavljenih znanstvenih prispevkov na konferencah
22 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 patent
1 predavanje na tuji univerzi
1 prispevek na konferenci brez natisa
1 vabljeno predavanje na konferenci brez natisa
2 končni poročili o rezultatih raziskav
2 diplomi

GLAVNI DOSEŽKI V LETU 2004

Zakaj v elektrokemijskih sistemih z adsorbiranimi produkti in/ali intermediati izmerimo negativne diferencialne upornosti in kapacitivnosti?

Že skoraj tri desetletja se v elektrokemijski literaturi pojavljajo številni izmerjeni impedančni spektri, kjer ima realni del impedance pri nizkih frekvencah negativno vrednost oziroma ima imaginarni del v določenem frekvenčnem območju pozitivno vrednost. Prvo značilnost avtorji pogosto pripisujejo obstoju »negativne diferencialne upornosti« v sistemu, drugo pa obstoju »negativne diferencialne kapacitivnosti« ali celo induktivnosti. Kvantitativna obravnava omenjenih značilnosti je presenetljivo redka. Le v dveh člankih so avtorji predlagali model, v katerem je eksplicitno podan izraz za omenjena »negativna« elementa, pa še v teh primerih gre za »kvazi« elementa, saj sta frekvenčno odvisna. Razvili smo model, v katerem prvič podajamo splošna izraza za frekvenčno neodvisno negativno diferencialno upornost in negativno

- Incorporation of funcctional materials into matrices;
- Influence of surface charge on stability of dispersions and suspensions; polyelectrolyte titrations.

BIBLIOGRAPHY

7 Original Scientific Articles
1 Professional Article
1 Popular Article
1 Other Article
1 Published Scientific Conference Contribution (Invited Lecture)
7 Published Scientific Conference Contributions
22 Published Scientific Conference Contribution Abstracts
1 Patent
1 Invited Lecture at a Foreign University
1 Unpublished Conference Contribution
1 Unpublished Invited Lecture at a Conference
2 Final Research Reports
2 Undergraduate Theses

IMPORTANT ACHIEVEMENTS IN 2004

Why the electrochemical systems with adsorbed products and/or intermediates exhibit negative differential resistances and capacitities?

Since the beginning of the electrochemical impedance measurements, the measured spectra have often exhibited unusual features such as negative values of the real part at low frequencies or positive values of the imaginary part in certain frequency range. The former feature has often been ascribed to a negative differential resistance within the system, while the latter has been explained in terms of a negative differential capacitance or, even, an inductance. Quantitative treatment of these - rather frequently observed - phenomena has been surprisingly rare. Only two papers have proposed models containing a formal description of such »negative elements«. However, in these models the elements could not be considered true

diferencialno kapacitivnost v elektrokemijskih sistemih z adsorbiranimi produkti in / ali adsorbiranimi intermediati. Za preprostejše primere model natančno pojasni fizikalno - kemijski vzrok za negativni predznak obeh elementov. Denimo negativna upornost je običajno posledica povečanega blokiranja površine s produkti, in s tem zmanjšanega toka, pri povečanem potencialu. Negativna kapacitivnost ima lahko različne vzroke, vedno pa gre za veličino, ki je neposredno sklopljena s »pravo« (pričakovano) kapacitivnostjo zaradi adsorpcije intermediatov / produktov elektrokemijske reakcije. Ker je izvor in sklopitev obeh tipov »faradejskih« kapacitivnosti zdaj znana, je postala možna tudi kvantitativna definicija tako imenovane »psevdokapacitivnosti«.

Gorivne celice: vpliv halogenidov na elektro-oksidacijo CO na platini

Eden od najbolj perečih in nerešenih problemov nizkotemperaturnih gorivnih celic je postopna zastrupitev platinskega katalizatorja s CO, ki je v majhnih količinah vedno primešan gorivu. Problem bi lahko elegantno rešili s pripravo modificiranih platinskih ali sorodnih katalizatorjev, na katerih bi oksidacija CO potekala v območju potencialov, kjer se sicer oksidira gorivo (vodik); s tem bi dosedanji strup pravzaprav postal dodatno gorivo. Da bo ta cilj zelo težko doseči, je potrdila tudi naša raziskava, v kateri smo sistematično proučili vpliv halogenidov in nečistoč v elektrolitu (nafionu) na oksidacijo CO. Prisotnost halogenidov v gorivni celici je namreč pogosta, saj mnogi sintezni postopki za pripravo katalizatorjev izhajajo prav iz halogenidov žlahtnih kovin. Izkazalo se je, da lahko že zelo majhna vsebnost halogenidov (10^{-5} mol/L) v elektrolitu premakne oksidacijo CO za okoli 100 mV proti pozitivnim potencialom, torej v obratno smer od želene. Z večanjem koncentracije halogenidov se njihov negativni učinek le še poveča. Halogenidi s površine katalizatorja namreč izpodrinejo vodo, ki je izvor »kisika«, potrebnega za elektro-oksidacijo CO. Podoben vpliv

equivalent - circuit elements as they were frequency dependent.

We have developed a new model containing true negative differential elements for electrochemical systems with adsorbed products or intermediates. In simpler cases, the model offers a clear physical-chemical explanation for both the negative resistance and the negative capacitance. For example, the negative resistance occurs in cases when at more positive potentials the metal surface is progressively blocked with intermediates, thus decreasing the current through the interface. The negative capacitance may have different physical - chemical origins but in all cases it seems to be coupled to another capacitance - the true (positive) capacitance due to adsorption of intermediates. Knowing the origin of and the coupling between both faradaic capacitances, it has now become possible to define quantitatively another frequently observed phenomenon - the so - called pseudocapcitance.

Fuel cells: influence of halogenides on electro-oxidation of CO on platinum

One of the crucial and still unsolved problems of low-temperature fuel cells is the gradual poisoning of platinum catalyst with CO, a substance that is always present in the fuel. An elegant solution of the problem would be preparation of modified platinum-based or similar catalyst on which the electrooxidation of CO and fuel oxidation would take place in the same potential region. This way, the present poison (CO) would actually serve as additional fuel. There are, however, many obstacles to achieving this goal. One has been demonstrated in our recent experiments in which we systematically studied the influence of halogenides and electrolyte impurities on CO electrooxidation. Namely, halogenides are inherently present in fuel cells as they are used as precursors in the synthesis of catalysts. We have found that already small concentrations of halides (10^{-5} mol/L) in electrolyte result in a 100 mV-shift of CO oxidation to positive potentials - that is, away

na elektro - oksidacijo CO imajo - za zdaj še neznane - nečistoče, ki jih pri sintezi vnesemo v nafion, torej najpogostejši elektrolit, ki se uporablja v PEM gorivnih celicah.

Elektrokemijsko ožičenje aktivnih delcev v bateriji: vloga ogljikovega filma
Trdni aktivni delci, ki shranjujejo naboj v bateriji, so najpogosteje slabi ionski in elektronski prevodniki. Ker so oboji nosilci naboja bistveni za elektrokemijsko aktivnost, moramo pri pripravi elektrod poskrbeti, da do vsakega aktivnega delca vodi ustrezen ionski in, hkrati, elektronski prevodnik. Pokazali smo, da je v primerih, ko so aktivni delci zelo majhni (500 nm ali manj), najprimernejši elektronski vodnik tanek ogljikov film, ki ga nanesemo na površino vsakega aktivnega delca. Ker je elektronska prevodnost sorazmerna z debelino filma, je na prvi pogled presenetljivo, da baterija bolje deluje, če je prevodni film zelo tanek (denimo 1-2 nm), kot če je nekoliko debelejši (3-5 nm). Pojav razložimo s tem, da je tanjši film bolj prepusten za ione v elektrolitu, ki v bateriji obdaja oplaščene aktivne delce. Povedano drugače: tanek ogljikov film, v kombinaciji z elektrolitom, vodi do boljše mešane prevodnosti kot debel film. Ugotovitev je izjemnega pomena za nadaljnji razvoj tehnologije oplaščevanja v novih generacijah baterijskih sistemov, ki temeljijo na uporabi nanostrukturiranih aktivnih materialov.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Iskra Baterije Zmaj d.d., Šentvid pri Stični; optimizacija baterijskih elektrod
- Belinka d.d., Ljubljana; študij stabilnosti barvnih suspenzij
- Lek d.d., Ljubljana; priprava kompozitov s kontroliranim sproščanjem učinkovin
- Predilnica Litija d.d., Litija; partner v Centru odličnosti Nanoznanosti in nanotehnologije, ESRR, ukrep 1.1 in 1.4
- Atotech Podnart d.d., Podnart; partner v Cen-

from the region of fuel (hydrogen) oxidation. The higher the halide concentration the more pronounced is the shift. The reason for the potential shift is the displacement of water from the catalyst surface by the halides; water, however, is the source of oxygen needed for CO electrooxidation. A similar »negative« influence on CO electrooxidation has been found for impurities that are present in nafion - the most frequently used electrolyte for PEMFC.

Electrochemical wiring of active particles in batteries: the role of carbon coatings
In a modern battery, charge is stored within solid particles which, however, by nature, exhibit rather poor ionic and electronic conductivity. As both types of charge are essential for electrochemical activity, it is necessary to create appropriate ionic and electronic paths to each active particle. We have shown that when active particles are smaller than ca 500 nm, an efficient way of creating electronic paths is preparation of thin carbon coatings around each particle. As electron conductivity is proportional to the thickness of coating, it might seem surprising that 1-2 nm thick coatings gave significantly better electrochemical performance than twice or three times thicker coatings. We explain this result by assuming that thinner coatings have much better permeability for lithium ions that, during operation, penetrate from the electrolyte surrounding the particles through the carbon layer into the active particle. In other words, although thinner carbon layers are poorer electronic conductors, they are the better choice for preparation of interfacial structures requiring mixed conductivity. This finding will serve as an important guideline for preparation of new generations of nanostructured battery materials.

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

- Iskra Batteries Zmaj d.d., Šentvid pri Stični, Slovenia; optimisation of battery electrodes

tru odličnosti Nanoznanosti in nanotehnologije, ESRR, ukrep 1.1 in 1.4

MEDNARODNO SODELOVANJE
- APOLLON, projekt v 5. okvirnem programu EU
- ALISTORE, mreža odličnosti v 6. okvirnem programu EU

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

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA
Mentorstva pri diplomah:
- Djordje Dmitrašinović; Priprava kompozitov SiO_2 -klaritromicin za prirejeno sproščanje (Fakulteta za farmacijo, Ljubljana, M. Gaberšček: somentor)
- Krešimir Grgić; Vpliv pomožnih snovi na raztapljanje naproksena po obarjanju iz zmesi topil (Fakulteta za farmacijo, Ljubljana, M. Bele: somentor)

Obiski tujih raziskovalcev:
- Frederic Sauvage, Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie, Amiens, Francija
- Fanny Barde, Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie, Amiens, Francija
- Dominique Larcher, Laboratoire de Réactivité et de Chimie des Solides, Université de
- Belinka d.d., Ljubljana, Slovenia; stability of paint suspensions
- Lek d.d., Ljubljana, Slovenia; composites with controlled release of drugs
- Predilnica Litija d.d., Litija, Slovenia; partner in Nanosciences and Nanotechnologies Centre of Excellence
- Atotech Podnart d.d., Podnart, Slovenia; partner in Nanosciences and Nanotechnologies Centre of Excellence

INTERNATIONAL COLLABORATION
- APOLLON, 5th EU Framework project
- ALISTORE, 6th EU Framework Network of Excellence

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

EDUCATION AND IMPORTANT VISITS
Mentors:
- Djordje Dmitrašinović; Preparation of SiO_2 - clarythromycin composites for controlled release (Undergraduate thesis, Faculty of Pharmacy, Ljubljana, M. Gaberšček: comentor)
- Krešimir Grgić; The influence of additives on dissolution of naproxen after the precipitation from mixture of solvents (Undergraduate thesis, Faculty of Pharmacy, Ljubljana, M. Bele: comentor)

Visits of foreign researchers:
- Frederic Sauvage, Laboratoire de Réactivité et de Chimie des Solides, Université de Picar-

Picardie, Amiens, Francija

Gostovanja:
- Robert Dominko na Université de Picardie, Amiens, Francija
- Janko Jamnik na Max-Planck-Institutu für Festkörperforschung, Stuttgard, Nemčija

7th INTERNATIONAL SYMPOSIUM ON SYSTEMS WITH FAST IONIC TRANSPORT

V mesecu maju so sodelavci L10 na Bledu organizirali odmevno mednarodno konferenco s področja trdnih ionskih prevodnikov (7th ISSFIT, www.issfit.ki.si). Eden od ciljev konference je bil soočiti najboljše zahodne strokovnjake z vrhunskimi kolegi iz bivšega "vzhodnega bloka", ki običajno nimajo možnosti sodelovati na, zanje, cenovno nedostopnih "zahodnih" konferencah. V ta namen je laboratorij sponzoriral udeležbo več kot 10 udeležencev. Kaže, da je bil zastavljeni cilj dosežen: konference se je udeležilo 80 udeležencev iz kar 25 različnih držav, med njimi iz 11 "vzhodnih". Ob poslušanju več kot 20 izvrstnih predavanj se je potrdila domneva, da kvalitete raziskav ne določa geografska lega, ampak - očitno - izvrstni posamezniki, ki jih - prav tako očitno - ne motivira denar, ampak predvsem radovednost.

die, Amiens, France
- Fanny Barde, Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie, Amiens, France
- Dominique Larcher, Laboratoire de Réactivité et de Chimie des Solides, Université de Picardie, Amiens, France

Visits of foreign institutes:
- Robert Dominko visited Université de Picardie, Amiens, France
- Janko Jamnik visited Max-Planck-Institut für Festkörperforschung, Stuttgard, Germany

7th INTERNATIONAL SYMPOSIUM ON SYSTEMS WITH FAST IONIC TRANSPORT

In May 2004, the coworkers of the Laboratory organized an international conference covering the field of solid ion and mixed conductors (7th ISSFIT, www.issfit.ki.si). An important goal was to confront the best researchers from the "West" with the most enthusiastic and inventive colleagues from the "East" who, mostly due to financial reasons, seldom get opportunity to participate at international conferences. For these purposes the Laboratory sponsored participation of more than 10 distinguished researchers from the East. It seems that the goal was reached: the conference was attended by 80 participants from 25 different countries, of that from 11 "eastern" countries. Listening to more than 30 excellent lectures has confirmed that the quality of research is not determined by geographical site but, obviously, by excellent individuals who are primarily motivated by curiosity rather than by finances.

SLIKA 2
Utrinek s konference 7th ISSFIT

FIGURE 2
Poster session at 7th ISSFIT

L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation

VODJA / HEAD
Prof. dr. Radovan Komel

RAZISKOVALCI / RESEARCHERS
Dr. Aleksandra Comino
Dr. Marija Anžur Lasnik (LEK)
Dr. Vladimira Gaberc Porekar
Dr. Simona Jevševar (LEK)
Dr. Nada Kraševec
Dr. Viktor Menart (KI / LEK)
Barbara Podobnik (LEK)
Dr. Marjetka Podobnik
Mag. Tatjana Vasle Preradov

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Mag. Apolonija Bedina Zavec
Petra Draškovič
Irena Fonda
Gorazd Hribar
Maja Kenig (LEK)
Mateja Kusterle (LEK)
Ljerka Lah
Ana Lenassi
Mateja Novak Štagoj
Špela Peternel
Matjaž Vogelsang

TEHNIČNO OSEBJE / TECHNICAL STAFF
Karmen Čerkič (LEK)
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Jelka Lenarčič
Nataša Lileg Tašler
Mateja Skok (LEK)
Tea Tomšič

GOSTUJOČI RAZISKOVALEC / VISITING SCIENTIST
Vanja Smilović

PODROČJA DEJAVNOSTI

Raziskave laboratorija L11 potekajo v okviru združenega programa med Kemijskim inštitutom ter Medicinsko in Veterinarsko fakulteto Univerze v Ljubljani, »Funkcijska genomika in biotehnologija za zdravje« (P1-0104), in treh raziskovalnih projektov: »Mikro in nano delci v biotehnologiji« (L4-6171) kot naslednik v letu 2004 zaključenega projekta »Razvoj TNF-alfa in analogov v terapiji raka« (L4-3324); »Steroidna 11beta-hidroksilaza iz nitaste glive *Cochliobolus lunatus*« (L4-4353); »Strukturne raziskave inozitol-polifosfatnih kinaz« (J4-6463).

Raziskovalni program sestavljajo naslednja področja:

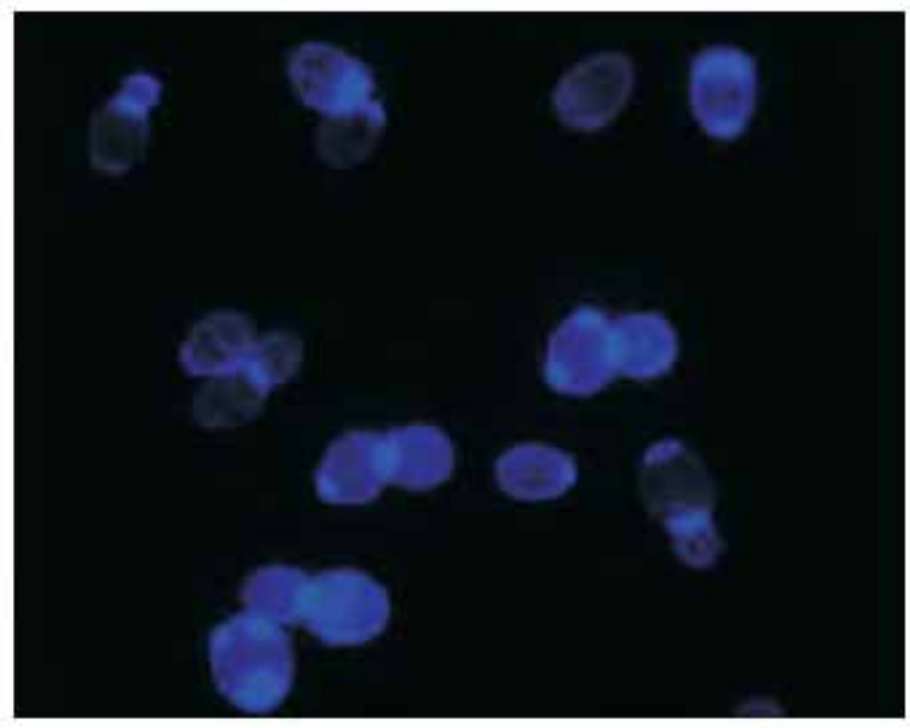
- Preučevanje metod za pridobivanje rekombinantnih citokinov
- Celična biologija kvasovke *S. cerevisiae*

RESEARCH ACTIVITIES

Research work of Laboratory L11 is accomplished through a multiparty research programme incorporating NIC, and Faculty of Medicine and Veterinary Faculty of the University of Ljubljana, Slovenia, as well as through three research projects. The research programme is entitled "Functional genomics and biotechnology for health" (P1-0104) and the research projects bear the following titles: "Micro and nano-particles in biotechnology" (L4-6171), "Steroid 11beta-hydroxylase from filamentous fungus *Cochliobolus lunatus*" (L4-4353) and "Structural studies of inositol polyphosphate kinases" (J4-6463).

Research programme of Laboratory L11 includes the following research areas:

- Investigation of approaches to biotechnological production of recombinant cytokines



SLIKA 1

Celice kvasovke *Saccharomyces cerevisiae*, pobarvane z barvilom kalkofluor belo.

SLIKA 1

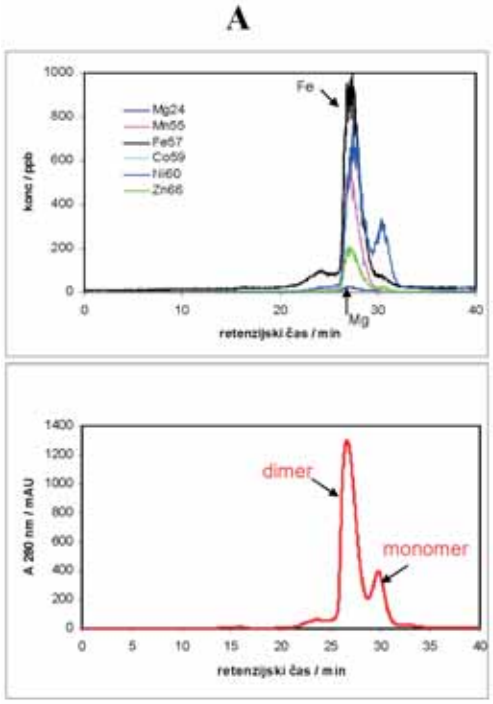
Saccharomyces cerevisiae cells stained by calcofluor white.

- Biotehnologija nižjih evkariontov (nitaste glive in kvasovke)
- Preučevanje in kloniranje genov za pretvorbe steroidov pri nitastih glivah
- Strukturne raziskave biološko aktivnih molekul.

Metodološki pristopi za izvajanje programa so:
- Gensko oziroma proteinsko inženirstvo: načrtovanje in pridobivanje novih, delno spremenjenih proteinskih molekul z izbolj-

- Cell biology of the yeast *Saccharomyces cerevisiae*
- Biotechnology of lower eucaryotes (filamentous fungi and yeasts)
- Study and gene cloning of steroid bioconverting enzymes in filamentous fungi
- Structural studies of biologically active molecules

Methodological approaches are as follows:
- Genetic and protein engineering: design and



B

element	m/z	konc (umol/L	RSD	+/- s (umol/L)
Mg	24	8,79	0.0716	0,41
Mn	55	47,9	0.0365	1,7
Fe	57	66,8	0.0542	3,6
Ni	60	1,74	0.0275	0,05
Zn	66	6,62	0.0633	0,42

Koncentracija proteina: 0.11 mM

C

element	m/z	konc (umol/L	RSD	+/- s (umol/L)
Mg	24	11,5	0.0664	0,77
Mn	55	69,5	0.0392	2,7
Fe	57	220	0.0299	6,6
Ni	60	22,1	0.0420	0,93
Zn	66	37,8	0.0554	2,1

Koncentracija proteina: 0.22mM

SLIKA 2

Kromatogram ločbe fosfodiesteraze iz bakterije *M. tuberculosis* na kromatografskem nosilcu Superdex 200.

A. Grafa prikazujeta absorpcijo proteina pri 280 nm ter ustrezno izmerjene vrednosti kovin v proteinu, izmerjene z ICP-MS.

B. Izmerjene vrednosti kovin na ICP-MS po totalnem razklopu vzorca, ki je bil predhodno obdelan s kelatorjema EDTA in DTT.

C. Izmerjene vrednosti kovin na ICP-MS po totalnem razklopu nativnega vzorca (brez kelatorjev). Prikazane so samo tiste kovine, ki so kazale signifikantne vrednosti koncentracij.

FIGURE 2

Elution profile of the phosphodiesterase from *M. tuberculosis* on Superdex 200 column.

A. Graphs show the protein absorption at 280 nm and the corresponding values for the metals present in the sample as measured by ICP-MS.

B. Metal content in the protein (mineralized samples) by ICP-MS (protein treated beforehand with the metal chelators EDTA and DTT).

C. Metal content in the protein (mineralized protein – no treatment with the metal chelators) by ICP-MS. Only metals showing the significant concentration values are shown.

šanimi lastnostmi za uporabo ali za lažje pridobivanje

- Proteinski laboratorij: izolacija, prečiščevanje in karakterizacija rekombinantnih proteinov
- Fermentacijska tehnologija: preučevanje osnovnih parametrov biosinteze s poudarkom na zakonitostih, ki veljajo za rekombinantne seve
- Celične kulture: gojenje sesalskih celičnih linij; uvajanje novih metod za testiranje biološke aktivnosti citokinov
- Genomika in proteomika: kvasni dvo - hibridni sistem za ugotavljanje celičnih interakcij »protein-DNA« oz. »protein - protein«, funkcijska analiza patogenih mutacij z uporabo kvasnih celic
- Lokalizacija celičnih proteinov s fluorescenčno mikroskopijo
- Preučevanje tri - dimenzionalnih struktur biološko aktivnih molekul z X-žarkovno kristalografijo in nuklearno magnetno resonanco (NMR)

BIBLIOGRAFIJA

12 izvirnih znanstvenih člankov
1 intervju
1 drug članek oz. sestavek
3 objavljeni znanstveni prispevki na konferencah (vabljena predavanja)
1 objavljen strokovni prispevek na konferenci
7 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 objavljen povzetek strokovnega prispevka na konferenci
5 patentov
6 diplom
1 magisterij
1 doktorat
2 uredništvi revij

DOSEŽKI V LETU 2004

- Pri raziskavah izražanja heterolognih genov v metilotrofni kvasovki *P. pastoris* so bili

production of novel, partially modified protein molecules with improved properties for final use or simplified isolation / purification

- Protein laboratory: isolation, purification and characterisation of recombinant proteins
- Fermentation technology: studies of basic parameters of biosynthesis, with an emphasis on the principles applicable for recombinant strains
- Cell cultures: cultivation of mammalian cell lines; introduction of new methods for biological activity testing of cytokines
- Genomics and proteomics: yeast two - hybrid system for studying cellular "protein-DNA" and "protein-protein" interactions; functional analysis of human gene mutations by yeast cell system
- Cellular localisation of proteins by fluorescence microscopy
- Three - dimensional structure determination of biologically active molecules by X-ray crystallography and nuclear magnetic resonance (NMR)

BIBLIOGRAPHY

12 Original Scientific Articles
1 Interview
1 Other Article
3 Published Scientific Conference Contributions (Invited Lectures)
1 Published Professional Conference Contribution
7 Published Scientific Conference Contribution Abstracts
1 Published Professional Conference Contribution Abstract
5 Patents
6 Undergraduate Theses
1 Master's Thesis
1 Doctoral Dissertation
2 Editorships

pripravljeni konstrukti za znotrajcelično izražanje in izločanje zelenofluorescirajočega proteina GFP, lahke verige goveje enterokinaze bEKL in topnega humanega receptorja shTNFR1 ter fuzijskih proteinov GFP-EKL-CH6 in GFP-TNFR1-CH6. V primeru sekretornih konstruktov po transformaciji v kvasovko *P. pastoris* GS115 na ploščah ni bilo zaslediti fluorescenčnih kolonij in v nobenem primeru tudi nismo zasledili prisotnosti ustreznih proteinov. V primeru znotrajceličnega izražanja pa smo na ploščah dobili fluorescenčne kolonije in dobre producente izbrali na osnovi jakosti fluorescence. Fuzijska proteina GFP-EKL-CH6 in GFP-TNFR1-CH6 predstavljata prvi primer znotrajcelične produkcije bEKL in shTNFR1. Oba fuzijska proteina flurescirata in to nakazuje, da se je GFP pravilno zvil, kar je omogočilo nastanek fluorofora. Oba fuzijska proteina se pojavljata v netopni frakciji, kjer zasledimo tudi encim alkoholna oksidaza AOX, ki je glavni peroksisomalni protein. Tako sklepamo, da je po vsej verjetnosti prišlo do vnosa fuzijskih proteinov v peroksisome. Za GFP je znano, da brez vodilnega zaporedja usmerja sekretorne proteine v vakuolo oziroma ER/Golgi. Naši poskusi pa kažejo, da je prosti N-konec GFP v fuzijskih proteinih odgovoren za usmerjanje proteinov v kvasne peroksisome, s čimer se nakazuje možnost uporabe teh organelov kot alternativnega produkcijskega sistema za tarčne proteine. Prednost peroksisomov je v njihovi veliki kapaciteti, ki omogoča kopičenje visokih količin nastalega proteina, ter v zaščiti proteinov pred celično proteolitsko razgradnjo.

- V letu 2004 smo nadaljevali raziskave mehanizmov delovanja nekaterih sistemsko manj toksičnih analogov TNF, saj bi poznavanje in razumevanje teh mehanizmov v prihodnosti lahko omogočilo usmerjeno načrtovanje in oblikovanje novih analogov s še boljšimi lastnostmi za terapijo različnih malignih obolenj. Na površini različnih endotelijskih celic smo po stimulaciji z

RESULTS IN 2004

- Expression studies of heterologous genes in methylotrophic yeast *P. pastoris* yielded numerous constructs for intracellular expression and secretion of the following proteins: green fluorescent protein GFP, light chain of bovine enterokinase bEKL, soluble human receptor shTNFR1 and two fusion proteins, GFP-EKL-CH6 and GFP-TNFR1-CH6. After transformation into *P. pastoris* GS115, in the case of secretory constructs no fluorescent colonies were obtained on agar plates and no respective proteins detected. In contrast, intracellular expression yielded fluorescent colonies enabling efficient selection of good producers on the fluorescence basis. Fusion proteins GFP-EKL-CH6 and GFP-TNFR1-CH6 represent the first example of intracellular biosynthesis of bEKL and shTNFR1 in *P. pastoris*. Both fusion proteins are fluorescent indicating that GFP was correctly folded enabling the formation of the characteristic internal fluorophor. Both fusion proteins were found in the insoluble fraction together with enzyme AOX (alcohol oxidase), which is the principal peroxysomal protein. This indicates that the fusion proteins are most probably imported into peroxysomes. It has already been reported that GFP itself, without any leading sequence, is capable of directing the secretory proteins into vacuoles and ER/Golgi, respectively. Our experiments have brought further evidence that the N-terminus of GFP in the fusion proteins is responsible for targeting into peroxysomes, exhibiting the capability of peroxisomes as an alternative production system with an advantage of accumulating high quantities of the target protein protected from proteolytic degradation.
- In 2004 mechanisms of action of some systemically less toxic TNF analogues were further investigated. Understanding of these mechanisms could lead to more targeted design of new TNF analogues possessing further improved properties for therapy of different forms of cancer. After stimulation of

različnimi proteini TNF določili ravni adhezijskih molekul ICAM-1, VCAM-1 in E-selektin. Ugotovili smo, da pri analogih dN6TNF, LK-805 in dN6LK-805 kljub povišanju specifične citotoksične aktivnosti *in vitro* ni prišlo do povišanja ekspresije adhezijskih molekul glede na nativen TNF. Poleg tega smo na modelu čistih tumorskih celic SA-1 dokazali, da imata tako TNF kot tudi analog LK-805 *in vitro* neposreden citotoksičen učinek na te tumorske celice. Dokazali smo tudi, da z inhibicijo transkripcijskega faktorja NF-kB povečamo občutljivost nekaterih tumorskih celic na terapijo s TNF in njegovimi analogi.

- V okviru projekta »Strukturne raziskave inozitol polifosfatnih kinaz«, ki poteka v povezavi z laboratorijem prof. Solomona H. Snyderja z Johns Hopkins Univeristy School of Medicine, Baltimore, ZDA, smo izdelali postopek za ekspresijo ter izolacijo večjih količin inozitol heksakis fosfat kinaze. Očiščeni encim ima visoko specifično aktivnost in je tudi zelo stabilen. V teku so priprave (z genskim kloniranjem) izoform inozitol heksakis fosfat kinaze, njihova ekspresija ter izolacija. Izolirano kinazo tudi kristaliziramo. Pripravljamo tudi eksperimente za analizo produktov encimske reakcije naše kinaze s pomočjo NMR (sodelovanje z NMR centrom KI) in masne spektroskopije (sodelovanje z laboratorijem za analizno kemijo KI).
- V sredini leta 2004 smo pričeli z raziskavami v okviru projekta »Strukturne študije cAMP fosfodiesteraze iz bakterije *M. tuberculosis*«, ki poteka v povezavi z laboratorijem prof. Sandhye Visweswariah z Indian Institute of Science, Bangalore, Indija. V preteklem letu smo ugotovili več zanimivih strukturnih posebnosti tega encima. Ugotovili smo, da se izraža večinoma v obliki dimera in da pride do delne cepitve, kar pa ne moti tvorbe dimerov. Položaj cepitve smo določili z N-terminalnim sekvenciranjem in masno spektrometrijo fragmentov, nastalih po proteolizni cepitvi. Protein je metalo-encim

various endothelial cells with TNF and its analogues, the expression levels of cell-surface adhesion molecules ICAM-1, VCAM-1 and E-selectin were determined. In the case of analogues dN6TNF, LK-805 and dN6LK-805, all possessing higher *in vitro* cytotoxic activities than TNF, no increase in expression of adhesion molecules was observed. Interestingly, on SA-1 tumour cell in vitro model direct cytotoxic effects of TNF or LK-805 were confirmed. Evidence was also provided that inhibition of the transcription factor NF-kB results in higher sensitivity of some tumour cell lines against TNF or its analogues.

- In collaboration with our industrial partner Lek Pharmaceuticals d.d., Ljubljana, Slovenia, new technologies for the production of the second - generation protein pharmaceuticals have been introduced. In 2004 some novel protein conjugates were prepared, purified and labelled for animal testing. During pharmacokinetic profile screening on rat for three of the tested conjugates a promising pharmacokinetic behaviour was confirmed, similar to an already existing successful market product. The respective conjugates have thus been qualified for further testing on monkeys.
- The project »Structural studies of the inositol poly-phosphate kinases« is running in collaboration with the research group of Prof. Solomon H. Snyder from the Johns Hopkins University School of Medicine, Baltimore, USA. In 2004 we have developed a large - scale expression and purification procedure for the inositol hexakisphosphate kinase. The purified enzyme is exhibiting high specific activity and is very stable. Cloning, expression and purification of some isoforms of the kinase are in progress, as well as the crystallization of the purified enzyme. The experiments to study the structures of the products produced in the kinase reaction, where we will use NMR (collaboration with the NMR center at NIC) and mass spectroscopy (Analytical Chemistry Laboratory at NIC), are also in progress.

in z Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) (sodelovanje z Laboratorijem za analizno kemijo na KI) smo pokazali, da v aktivnem mestu vsebuje železo in mangan. Izdelali smo tudi metodo za ekspresijo ter izolacijo tega encima v večjih količinah iz *E. coli*. Encim tudi kristaliziramo.

- V sodelovanju z našim industrijskim partnerjem, Farmacevtsko družbo Lek d.d., Ljubljana, smo osvojili nove tehnologije za pridobivanje proteinskih farmacevtikov druge generacije. V letu 2004 smo pridobili nekaj lastnih konjugiranih proteinov, ki smo jih prečistili in označili za testiranje na živalskih modelih. Nekateri od testiranih konjugatov so v presejalnih testih na podganah pokazali podobno farmakokinetično obnašanje, kot ga kaže uspešen tržni produkt, in so se tako kvalificirali za nadaljnje poskuse na človeku podobnih opicah.
- V sklopu raziskav celičnega cikla pri kvasovki S. cerevisiae smo nadaljevali študij sumoilacije proteina Ecm11. Z *in situ* mutagenezo smo proteinu Ecm11 spremenili dve potencialni sumoilacijski mesti K5 in K103 tako, da smo aminokislino lizin zamenjali z argininom. Nobena od zamenjav ni vplivala na občutljivost seva na kalkofluor belo, ki je sicer značilna za seve z uničenim genom ECM11. Funkcija, ki jo ima Ecm11 med procesom mejoze, pa je povsem odvisna od sumoilacije na mestu K5. Raven nastanka askusov pri sevu Ecm11K5N je bila enaka kot pri sevu z uničenim genom ECM11. Spremenjeno mesto K103N ni imelo nikakršnega učinka na mejozo. Naši rezultati so pokazali, da je sumoilacija regulatorni mehanizem v procesu mejoze in da se protein Ecm11 sumoilira na mestu K5. Vpliv Ecm11 na organizacijo celične stene pa ni bil odvisen od sumoilacije. Ugotovili smo tudi, da proces sporulacije pri sevih z izničenim genom ECM11
- In the summer 2004 the project "Structural Studies of cAMP phosphodiesterase from *M. tuberculosis*" was started in collaboration with the research group of Prof. Sandhya Visweswariah from the Indian Institute of Science, Bangalore, India. The studies have revealed various interesting structural properties of the enzyme. We have shown that phosphodiesterase from *M. tuberculosis* is expressed mainly as a dimer. The protein is partially nicked, which however doesn't disturb the dimer formation. The position of the proteolytic cleavage was determined by N-terminal sequencing and mass spectrometry of the nicked protein. Protein is a metallo - enzyme. The presence of iron and manganese in the active site was shown by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) (collaboration with the Analytical Chemistry Laboratory at NIC). We have also developed a large - scale expression and purification protocol for this enzyme. Crystallization of the phosphodiesterase is in progress.
- Studies of *S. cerevisiae* cell cycle were focused on sumoylation of the Ecm11 protein. Two potential sumoylation sites K5 and K103 were mutated to arginine residues but these mutations did not alter the strain susceptibility against calcofluor white, the typical characteristics of strains with an extinguished ECM11 gene. The Ecm11 function during meiosis was found to entirely depend on K5 sumoylation, but not on K103 sumoylation. The level of asci formation was similar in the Ecm11K5N strain and the strain with ECM11 gene knocked out. Our results demonstrate that sumoylation represents an important regulatory mechanism in the process of meiosis, Ecm11 being sumoylated at K5. However, Ecm11 effect on cell wall organization is sumoylation independent. Sporulation in strains with knocked out ECM11 was found to be approximately 20% lower than in the wild strains. In heterozygous strains somewhat higher percentage of asci was found than in homozygous strains ecm11D. Further-

zaostaja glede na sporulacijo divjih sevov in da je pri njih končni procent nastalih askusov za 20% nižji. Heterozigotni sevi tvorijo nekoliko večji procent askusov kot homozigotni sevi ecm11D, sevi divjega tipa z dodatno kopijo ECM11 na plazmidu pa imajo manjšo učinkovitost sporulacije kot sevi divjega tipa. Očitno so kvasovke občutljive na število genov ECM11 v celici in je ekspresija tega gena zelo natančno uravnavana. Heterozigotnemu sevu in sevu divjega tipa z dodatno kopijo ECM11 na plazmidu smo izmerili količino DNA med procesom mejotične replikacije in ugotovili, da ta pri teh sevih poteka enako kot pri sevu divjega tipa. Meritve ravni rekombinacije med mejozo so pokazale, da je pri heterozigotnem sevu raven konverzije genov nekje med obema sevoma: ecm11D in divjim tipom. Divji sev z dodatno kopijo ECM11 na plazmidu pa ima nekoliko višjo raven konverzije genov kot sam izvorni sev.

- Ker postajajo metode za preiskovanje in obvladovanje velikega števila parametrov in podatkov v moderni biotehnologiji vse bolj pomembne, smo razvili in optimirali lastno analitsko metodo za kvantitativno preiskovanje velikega števila različnih kvasnih mutant *in vivo*. V procesu sinteze heterolognih proteinov iz promotorja GAL1 sodelujejo številni geni oziroma njihovi produkti. Predvidevali smo, da izničenje nekaterih genov, ki so ključni za sintezo (transkripcijski dejavnik Gal4p; regulatorne molekule Gal3p, Gal80p; gradbene molekule kompleksa SAGA, metabolni encimi, ki sodelujejo pri razgradnji induktorja) bodisi popolnoma ali le deloma zavrejo heterologno ekspresijo ali pa jo celo izboljšajo. Hipotezo smo preverili in dokazali s pomočjo hitre, enostavne in točne kvantitativne metode, ki je omogočila spremljanje ravni heterologne ekspresije v velikem številu mutiranih sevov *Saccharomyces cerevisiae*. Metoda temelji na merjenju fluorescence zeleno-fluorescirajočega proteina GFP v živih celicah na mikrotitrskih

more, additional copy of ECM11 on the plasmid also resulted in lower capability of sporulation as compared to the wild strain. Yeasts are obviously susceptible to the number of ECM11 genes per cell and the respective gene expression is precisely regulated. During meiotic replication very similar DNA levels were found for heterozygous, wild type strain, and wild type strain with an extra copy of ECM11. Gene conversion level of heterozygous strain was found to be intermediate between the ecm11D and the wild strain, while the wild strain bearing an extra ECM11 copy possessed somehow higher gene conversion level than the wild strain itself.

- In modern biotechnology, methods for screening and manipulating a great number of parameters and data are becoming more and more important, therefore a novel analytical method for quantitative screening of a large number of different yeast mutants was developed and optimized. In the process of synthesis of heterologous proteins by GAL1 promoter numerous genes are involved. Our hypothesis was that knock - out of specific genes, important for the synthesis (transcription factor Gal4p; regulatory molecules Gal3p, Gal80p; building molecules of SAGA complex, metabolic enzymes involved in degradation of inducer) would either completely or partially destroy heterologous expression or, in contrast, could even accelerate it. The idea was checked and confirmed using a quick, simple and accurate quantitative method that enables monitoring of heterologous expression level for a large number of mutated *S. cerevisiae* strains. The method is based on fluorescence measurement of GFP in the living cells on micro-titer plates. In mutant strains with inactivated genes that are directly or indirectly involved in regulation of GAL1 promoter, the level of reporter GFP molecule was determined. Gal1 and Gal4 were found as the most important proteins

ploščicah. Določili smo raven poročevalske molekule GFP v mutiranih sevih, ki imajo inaktivirane gene, ki so neposredno ali posredno vključeni v regulacijo promotorja GAL1. Ugotovili smo, da sta za ekspresijo iz promotorja GAL1 najpomembnejša proteina Gal1 in Gal4. Konstruirali smo rekombinantni sev *S. cerevisiae* in z metodo "delitto perfetto" na kromosomu II zamenjali dva gena, ki sta vključena v proces sinteze proteinov iz promotorjev GAL. Dosegli smo bistveno izboljšanje specifične produktivnosti rekombinatnih proteinov. Z dobljenimi rezultati smo dodatno prispevali k razumevanju vpliva mnogih genskih produktov, vključenih v uravnavanje sistema GAL.

- V letu 2004 smo iz genomske knjižnice nitaste glive *Cochliobolus lunatus* uspeli izolirati gensko sekvenco 500 a.k. dolgega zaporedja, ki po primerjavi podatkov iz BLAST sodi v družino citokromov CYP53. Proteinu, ki kaže 62-65% identičnost s poznanimi citokromi P450, smo določili strukturne domene, ga uvrstili v dendrogram in v sodelovanju s strukturnimi biokemiki Medicinske fakultete Univerze v Ljubljani izdelali računalniški model njegove 3D-strukture. Protein bomo izrazili v *E.coli*, opravili njegovo funkcijsko analizo in ga poskusili kristalizirati za nadaljnje strukturne raziskave. Uspelo nam je izolirati tudi skoraj celotno gensko sekvenco ene od obeh predpostavljenih citokrom P450 reduktaz, v tem primeru CPR1 (manjka sekvenca 100 a.k. na začetku proteina) in delno, framentirano zaporedje druge predpostavljene reduktaze, CPR2. Z različnimi PCR-pristopi oz. s Southernovo analizo genomskih knjižnic bomo poskusili izolirati oba produkta in nato rekonstituirati hidroksilazni encimski sistem v celoti. V nadaljevanju raziskave bi z ugotavljanjem strukturnih razlik med citokromi gostiteljskih organizmov (rastline, človek) in citokromi nitaste glive *C.lunatus* poskušali poiskati "šibke točke" glivnih citokromov - kot osnove za načrtovanje njihovih inhibitorjev. Gliva *C.lunatus* je namreč

for expression by GAL1. A recombinant *S. cerevisiae* strain was constructed, and using a "delitto perfetto" method, on chromosome II two genes responsible for protein synthesis by GAL promoter were mutated resulting in essentially improved specific productivity of recombinant proteins. Our results contribute to understanding of functioning of a number of gene products, engaged in GAL system regulation.

- In 2004 we isolated from genomic library of the filamentous fungus *Cochliobolus lunatus* a gene sequence coding for a 500 amino acid protein that by BLAST search belonged to CYP53 family, showing 62-65% identity with different cytochromes P450. Structural domains of the protein were assigned, the dendograme proposed, and the computer model of its 3D structure was elaborated. Expression of the protein in *E.coli* is in progress for its functional analysis and structural studies. In 2004 we also isolated partial gene sequence of the putative cytochrome P450 reductase (CPR1) in which a nucleotide sequence that encodes the first 100 amino acids from the N-terminus is still lacking. Furthermore, we isolated also partial, fragmentised gene sequence of the second putative reductase, CPR2. Both genes will be determined by screening *C.lunatus* genomic and cDNA libraries with Southern blot analysis in order to reconstitute the entire hydroxylating system of the fungus. By looking for structural differences between fungal cytochromes and those from the host organisms we will try to find "weak points" of the fungal cytochromes as the starting point for the design of inhibitors. Namely, *Cochliobolus lunatus* is plant and opportune human pathogen.
- In the frame of the call for interests for funding research and development through EC European Regional Development Fund (ERDF) as published by the Slovenian Ministry for Education, Science and Sports, together with

rastlinski patogen in oportuni človeški patogen.

- V letu 2004 smo, v okviru razpisa Ministrstva za šolstvo, znanost in šport in Ministrstva za gospodarstvo Republike Slovenije, za pridobitev sredstev ESRR, sestavili konzorcij 20 partnerjev iz dveh slovenskih univerz (Univerza v Ljubljani - Medicinska fakulteta, Biotehniška fakulteta, Fakulteta za farmacijo, Fakulteta za elektrotehniko, Fakulteta za računalništvo in informatiko, Veterinarska fakulteta; Univerza v Mariboru - Medicinska fakulteta), slovenskih raziskovalnih inštitutov (Kemijski inštitut, Institut Jožef Stefan, Nacionalni inštitut za biologijo), zdravstvenih ustanov (Zavod Republike Slovenije za transfuzijsko medicino), malih in srednjih podjetij (Celica d.o.o., Ljubljana; CREA d.o.o., Ljubljana; Educell d.o.o., Ljubljana; LUI d.o.o., Ljubljana) in obeh farmacevtskih družb (Farmacevtska družba Lek d.d., Ljubljana, član skupine Sandoz, in Krka, tovarna zdravil d.d., Novo mesto). Ustanovili smo medinstitucionalen center odličnosti (CO) "Biotehnologija s farmacijo" z dvema RR - projektoma: RR1 - Razvoj novih zdravil in bio - čipov; RR2 - Načrtovanje, pridobivanje in karakterizacija biofarmacevtikov. Nosilec in koordinator CO "Biotehnologija s farmacijo" je naša programska skupina oz. Medicinska fakulteta Univerze v Ljubljani, nosilca RR - projektov pa sta Fakulteta za farmacijo Univerze v Ljubljani (projekt RR1) in Kemijski inštitut oz. ponovno naša programska skupina (projekt RR2). CO je v oktobru 2004 tudi odobrila vlada Republike Slovenije in mu za izvajanje obeh RR - projektov dodelila finančna sredstva iz skladov ESRR (ukrep 1.1). Glavna namena CO sta: (a) povezati raziskave med slovenskimi raziskovalnimi ustanovami na področju nove, post - genomske biotehnologije in jih umestiti v razvojne perspektive slovenske farmacevtske industrije kot enega od najbolj propulzivnih elementov našega gospodarskega razvoja; in (b) v Slovenijo pridobiti infrastrukturo novega tehnološkega

the Ministry for Economy, we established a consortium of 20 partners from the Slovenian universities (University in Ljubljana - Faculty of Medicine (MF), Faculty of Pharmacy (FP), Biotechnical Faculty (BF), Electrotechnical Faculty, Faculty for Computer Sciences and Informatics, Veterinary Faculty; University in Maribor - Faculty of Medicine), research institutes (National Institute of Chemistry (NIC), Institute Jožef Stefan (IJS), National Institute of Biology), health care institution (Institute for Transfusion Medicine), S&M enterprises (Celica d.o.o., Ljubljana, Slovenia; CREA d.o.o., Ljubljana, Slovenia; Educell d.o.o., Ljubljana, Slovenia; LUI d.o.o., Ljubljana, Slovenia) and the pharmaceutical industry (Lek Pharmaceuticals d.d., Ljubljana, Slovenia - a member of the Group Sandoz; KRKA Pharmaceuticals d.d., Novo mesto, Slovenia), and its Centre of Excellence (CE) "Biotechnology With Pharmacy" presenting two R&D projects: RR1 - "Development of new pharmaceutics and bio - chips"; RR2 - "Design, production and characterization of biopharmaceutics", the second one being coordinated by our research laboratory. In October 2004 the CE was recognized by the Government as one of the eight Slovenian R&D centres of excellence and started to be funded by ERDF. There are two main objectives of the CE: (a) networking the research at the Slovenian research laboratories in the field of new, post-genomic biotechnology and linking this research to R&D perspectives of the Slovenian pharmaceutical industry as one of the main players of the national economical development; and (b) to install infrastructure of the new technological generation to open to Slovenian research community the way to post - genomic research on functional genomics and modern biotechnology as one of the most exposed priorities of the European science and economical & social development. In this context our CE is establishing the following fully interlinked and coordinated infrastructural centres: (1) bio - chip

vala za post - genomske raziskave na področju funkcijske genomike in nove biotehnologije kot ene od sedmih prioritet evropske znanosti in njenega gospodarsko - družbenega razvoja. CO "Biotehnologija s farmacijo" v tem pogledu predvideva ustanovitev naslednjih, med seboj povezanih in koordiniranih infrastrukturnih sklopov: (1) tehnologija biočipov (na Medicinski fakulteti Univerze v Ljubljani); (2) proteomika (na Institutu Jožef Stefan); (3) metabolomika (na Fakulteti za farmacijo Univerze v Ljubljani); (4) strukturna in celična biologija (na Kemijskem inštitutu); (5) transgeneza (na Biotehniški fakulteti Univerze v Ljubljani) in (6) molekularna celična fiziologija (na Medicinski fakulteti Univerze v Ljubljani). Ukrep 1.4 ESRR naj bi spodbudil izgradnjo omenjene infrastrukture, pri kateri Slovenija močno zaostaja za veliko večino držav članic EU.

SODELOVANJE Z INDUSTRIJO

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

MEDNARODNO SODELOVANJE

- Leta 1994 je bil na Kemijskem inštitutu ustanovljen virtualen Inštitut za molekularno biologijo in biotehnologijo, ki združuje biokemike, molekularne biologe in biotehnologe Kemijskega inštituta, Inštituta Jožef Stefan, Fakultete za kemijo in kemijsko tehnologijo ter Medicinske fakultete. Ta inštitut je slovenski Pridruženi center (Affiliated Centre) ICGEB (International Centre for Genetic Engineering and Biotechnology, Trst, Italija). To pomeni, da sta vodenje in koordiniranje Pridruženega centra locirani na KI pri Laboratoriju za biosintezo in biotransformacije (L11).
- National Institute for Biological Standards and Control (NIBSC), Potters Bar, Velika Britanija:

(microarray) technology (MF); (2) proteomics (IJS); (3) metabolomics (FP); (4) structural & cell biology (NIC); (5) transgenesis (BF); and (6) molecular cell physiology (MF). We believe that ERDF support will enable Slovenia to establish research infrastructure of the new technological generation in the way it was already done at the great majority of the EU countries, including the new member states.

INTERNATIONAL COLLABORATION

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

- In 1994 the Institute for Molecular Biology and Biotechnology incorporating biochemists, molecular biologists and bio - technologists of the National Institute of Chemistry, Jožef Stefan Institute, Faculty of Chemistry and Chemical Technology, and Medical Faculty was founded at the National Institute of Chemistry. The virtual Institute for Molecular Biology and Biotechnology represents the Slovenian Affiliated Centre of ICGEB (International Centre for Genetic Engineering and Biotechnology, Trieste, Italy). Thus, leadership and co-ordination of the Affiliated Centre are located at the Laboratory L11 at the National Institute of Chemistry.
- National Institute for Biological Standards and Control (NIBSC), Potters Bar, Great Britain: bilateral collaboration sponsored by the Ministry of High Education, Science and Technology of Slovenia and The British Council.
- Johns Hopkins University Medical School, Baltimore, USA: collaboration with Dr. Rashina Bhandari from the laboratory of Prof. Solomon Snyder on the project "Structural studies of inositol poly-phosphate kinases".
- Indian Institute of Science, Bangalore, India: collaboration with Prof. Sandhya Viswes-

bilateralno sodelovanje, sofinancirano s strani Ministrstva za visoko šolstvo, znanost in tehnologijo in Britanskega sveta.

- Johns Hopkins University Medical School, Baltimore, ZDA: sodelovanje z dr. Rashina Bhandari iz laboratorija prof. Solomona Snyderja na projektu "Strukturne raziskave inozitol polifosfatnih kinaz".
- Indian Institute of Science, Bangalore, Indija: sodelovanje s prof. Sandhya Visweswariah na projektu "Strukturne študije cAMP fosfodiesteraze iz *M. tuberculosis*".

POMEMBNEJŠI INŠTRUMENTI IN OPREMA

- Laboratorij za gensko tehnologijo
- Izotopski laboratorij za delo s ^{3}H, ^{32}P in ^{35}S
- Laboratorij za izolacijo, čiščenje in karakterizacijo (rekombinantnih) proteinov
- Laboratorij za celične kulture
- Mikrobiološki laboratorij
- Laboratorij z bioreaktorji

Vsi omenjeni laboratoriji so ustrezno opremljeni, kot pomembnejšo pa posebej navajamo naslednjo opremo: pretočni citometer z možnostjo sortiranja celic (Becton Coulter), fluorescenčni mikroskop (Zeiss - Jena) s sistemom za analizo slike, stereo mikroskop (Nikon), 4 preparativni sistemi za kromatografske separacije proteinov (Amersham Biosciences, Knauer), 1 analitski HPLC system (Waters), UV/VIS spektrofotometer (Hewlett Packard), fluorimeter (PTI), dva računalniško vodena laboratorijska bioreaktorja (Applikon), dva sistema za pripravo milliQ vode (Millipore), hladilne kapacitete $+4^{o}C$, $-20^{o}C$ in $-70^{o}C$ ter sklop aparatur za pomnoževanje in sekvenčno analizo DNA.

wariah on the project "Structural studies of cAMP phosphodiesterase from *M. tuberculosis*".

MAJOR EQUIPMENT

- Laboratory for gene technology
- Laboratory for isotopes: ^{3}H, ^{32}P and ^{35}S
- Laboratory for isolation, purification and characterisation of (recombinant) proteins
- Laboratory for cell cultures
- Laboratory for microbiology
- Laboratory with bio - reactors

All above laboratories are adequately equipped, just to mention some important pieces: flow cytometer with cell sorter (Becton Coulter), fluorescence microscope with an image analysis system (Zeiss - Jena), stereo microscope (Nikon), four preparative HPLC systems for protein separations (Amersham Biosciences, Knauer), analytical HPLC system (Waters), UV/VIS spectrophotometer (Hewlett Packard), fluorimeter (PTI), two computer assisted laboratory bio - reactors (Applikon), two systems for milliQ water (Millipore), cooling and freezing capacities ($+4^{0}C$, $-20^{0}C$ and $-70^{0}C$), set of instruments for PCR and DNA sequence analysis.

L12

Laboratorij za biotehnologijo

Laboratory of Biotechnology

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PRIPRAVNIKI / TRAINEES
Gabriela Panter
Suzana Mesojednik
Gregor Tevž

PODROČJA DEJAVNOSTI

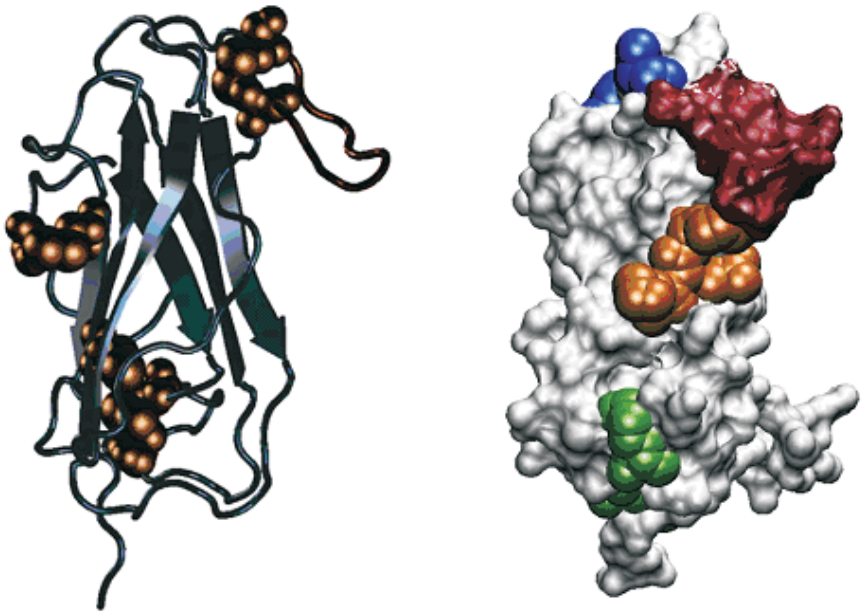
Raziskave v laboratoriju so usmerjene v raziskave bioloških procesov kot sta prepoznavanje bioloških makromolekul in prenos signalov v celicah in imajo potencialno uporabnost (predvsem biotehnološko, medicinsko, farmacevtsko). Pri tem uporabljamo moderne metode biokemije, molekularne biologije, mikrobiologije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

Raziskave s področja medicine se nanašajo na molekularne mehanizme sepse, konformacijskih bolezni in delovanja antimikrobnih učinkovin. Zanimajo nas mehanizmi prepoznavanja in biološke aktivnosti na molekularni ravni, zlasti molekulskih vzorcev značilnih za patogene mikroorganizme (PAMP), zato uporabljamo instrumentalne metode z visoko ločljivostjo in občutljivostjo, kot sta jedrska magnetna resonanca (NMR) in fluorescenčna spektroskopija. Raziskave vključujejo študij fiziologije

RESEARCH ACTIVITIES

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

Research topics with application in medicine are molecular mechanisms of sepsis, conformational disease and antimicrobial activity of (lipo)peptides. We are interested in the mechanism of recognition of pathogen associated molecular patterns (PAMPs) at the molecular level where we are employing methods with high resolution such as nuclear magnetic resonance and fluorescence spectroscopy. Research interests include study of metabolic regulation



SLIKA

Model 3D strukture človeškega MD-2 z označenimi disulfidi (rumene krogle, levo) in mutiranimi skupki bazičnih aminokislin ter gibljivo zanko med Cys95 in Cys105 (rdeča površina na desni sliki). (Gruber in sod., J.Biol.Chem. 2004).

FIGURE

Model of tertiary structure of human MD-2 with shown disulfides (yellow spheres, left panel) and mutated clusters of basic surface residues and flexible loop between Cys95 and Cys105 (red surface, right panel) (Gruber et al., J.Biol.Chem. 2004)

mikroorganizmov, ki izločajo encime, organske kisline, antibiotike in druge zdravilne učinkovine, kot tudi rekombinantne proteine. Laboratorij vzdržuje mikrobiološko zbirko (MZKI), v kateri hranimo več kot 3000 sevov mikroorganizmov, predvsem ekstremofilnih gliv in jo redno dopolnjujemo z novimi izolati.

BIBLIOGRAFSKI PODATKI

17 izvirnih znanstvenih člankov
2 samostojna znanstvena sestavka v monografijah
2 intervjuja
2 drugi učni gradivi
4 objavljeni znanstveni prispevki na konferencah (vabljeno predavanje)
1 objavljeni znanstveni prispevek na konferenci
35 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 objavljeni povzetek strokovnega prispevka na konferenci
1 patentna prijava
1 prispevek na konferenci brez natisa
1 končno poročilo o rezultatih raziskav
1 izvedensko mnenje
8 diplom
1 magisterij
2 uredništvi revij

GLAVNI DOSEŽKI V LETU 2004

- Na področju raziskav molekularnega mehanizma sepse smo se orientirali na protein MD-2, kjer kombiniramo strukturno in molekularno biologijo. V letu 2004 smo vzpostavili laboratorij za celične kulture in sistem za detekcijo celične aktivacije preko luminiscence, kar nam omogoča, da samostojno opravljamo vse raziskave, ki vključujejo odziv na celičnih kulturah. Objavili smo članek o modelu MD-2, kjer smo identificirali predele molekule, preko katerih poteka interakcija z LPS. Pripravili smo rekombinanten človeški MD-2 v *E.coli*, ki kljub temu da ni glikoziliran, omogoča celični odziv na LPS. MD-2 ima podobne biokemijske lastnosti kot alergen iz

in microorganisms, which are able to excrete a number of useful bioproducts, such as enzymes, organic acids, antibiotics and other pharmaceuticals, as well as recombinant proteins. Department hosts its own Microbial Culture Collection (MZKI), with more than 3000 different strains, with emphasis on extremophiles, which is regularly expanded by new species isolated from their natural environment.

BIBLIOGRAPHY

17 Original Scientific Articles
2 Scientific Articles in Monographs
2 Interviews
2 Other Educational Materials
4 Published Scientific Conference Contributions (Invited Lectures)
1 Published Scientific Conference Contribution
35 Published Scientific Conference Contribution Abstracts
1 Published Professional Conference Contribution Abstract
1 Patent Application
1 Unpublished Conference Contribution
1 Final Research Report
1 Expert Opinion
8 Undergraduate Theses
1 Master's Thesis
2 Editorships

IMPORTANT ACHIEVEMENTS IN 2004

- Research on the molecular mechanism of sepsis concentrated on protein MD-2, where we have combined structural and molecular biology. We have established a cell culture laboratory and a system for detection of cell activation through luminescence reporters, which allows us to perform independent research, involving response on cell cultures. We have published our results on the structural model of MD-2, where we have identified regions, which are involved in LPS recognition. We have prepared recombinant MD-2 in *E.coli*, which conferred, despite the lack of glycosylation, LPS responsiveness to

pršic Der p 2, na osnovi katerega smo postavili strukturni model MD-2. Na osnovi omenjenega proteina smo pripravili protitelesa kot reagent za detekcijo interakcij MD-2. V sodelovanju s skupino Raziskovalnega centra Borstel smo raziskali interakcijo proteina LALF z endotoksinom s pomočjo biofizikalnih metod.

- Nadaljevali smo z raziskavami peptidov, ki imajo antimikrobno delovanje in nevtralizirajo LPS. Analizirali smo drugo generacijo peptidov, ki so imeli bistveno izboljšano antimikrobno delovanje in smo jih zasnovali na osnovi 3D strukture peptidov v kompleksu z LPS in v micelah kot membranskih mimetikih. Ugotavljali smo vpliv acilacije peptida na spremembo aktivnosti in interakcijo z membranami ter njegovo 3D strukturo v zwitterionskih micelah.
- V okviru raziskav detekcije sprememb konformacije prionskih proteinov smo analizirali vezavo fluorescenčnih barvil, ki se vežejo na prionske proteine s spremenjeno konformacijo.
- Primerjava meritev kinetičnih parametrov med krajšim fragmentom in nativno fosfofruktokinazo (pfkA) je pokazala, da je pod fiziološkimi pogoji fragment zelo verjetno bolj aktiven, saj fruktoza-2,6-bifosfat kot aktivator nanj učinkuje dosti bolj stimulatorno. Pripravili smo pet različno dolgih genov pfkA, in sicer tako, da smo jim nukleotidno zaporedje krajšali s 3' konca. Po vnosu konstruktov v celice glive *A.niger* smo pri trasformantih merili PFK aktivnost po tem, ko smo umetno inducirali fosforilacijo z dodatkom azida. Pri sevu, ki je nosil skrajšan pfkA gen, ki je kodiral 450 amino kislinskih ostankov dolg protein, smo uspeli v homogenatu zaznati kinetiko karakteristično za krajši fragment. Gen za krajši fragment PFK smo poslali vsem partnerskim laboratorijem, s katerimi sodelujemo na projektu ANTICO, s ciljem, da ga vgradijo v druge komercialno zanimive mikroorganizme.

HEK293 cells transformed with TLR4. MD-2 has similar biochemical properties as mite allergen Der p 2, which was used as a template for the structural model of MD-2. In collaboration with a group at the Research Center Borstel we have investigated the interaction of endotoxin with a neutralizing protein (LALF) using biochemical and biophysical methods. We have continued the research of antimicrobial peptides, which neutralize LPS. We have designed and analyzed the second generation of peptides, which have significantly improved biological activity and have been designed based on tertiary structures of peptides in complex with LPS and micelles as membrane mimetics. The effect of peptide acylation on the activity, membrane interaction and 3D structure in micelles were investigated.

- In the framework of conformational changes of prion proteins we have analyzed binding of fluorescent probes, which bind to prion protein with modified conformation.
- Comparison of kinetic parameters between native phosphofructokinase and its shortened variant indicated that the fragment has most likely higher activity than native protein under physiological conditions, as the activator fructose-2,6-bisphosphate induces much higher activity. We have prepared 5 deletion variants of pfkA, shortened at their 3' end. After transformation of *A.niger* with constructs and phosphorylation has been induced by the addition of azide PFK activity was determined. Kinetic characteristic of the shortened variant in the strain transformed with variant, consisting of 450 residues was observed. A construct with the shortened variant was sent to the partner laboratories participating in the ANTICO project in order to incorporate it into other industrially interesting microorganisms.
- We have prepared recombinant pH sensor, which allows novel approach of measuring intracellular pH in filamentous fungi. Absorb-

- Pripravili smo rekombinantni pH senzor, ki omogoča nov pristop k merjenju intracelularnega pH pri filamentoznih glivah. Absorbanca in fluorescenca zeleno fluorescirajočega proteina je močno odvisna od vrednosti pH. Pripravili smo novo varianto GFP imenovano RaVe_C in ga izrazili v glivi *Aspergillus niger.* Konstanta RaVe_C pKa je 6.9 in je idealna za spremljanje pH sprememb v citosolu. Karakteristike biosenzorja pri *A.niger* smo analizirali z uporabo konfokalnega laserskega mikroskopa, pri tem smo potrdili, da je ekspresija RaVe_C zadostna za upodabljanje in da se biosenzor odziva na znotrajcelične spremembe pH.
- Na področju raziskav biotehnološke uporabnosti gliv in njihovih encimov smo proučevali zlasti oksidativno sposobnost za razbarvanje melaninov in sintetičnih organskih barvil ter zmožnost razgradnje sintetičnega polimera poliamida-6. V sodelovanju s tujimi partnerji smo nadaljevali raziskave predhodno pridobljenih proteolitičnih encimov glede uporabnosti za farmacevtske namene, hidrolizo proteinov in za biotransformacije organskih spojin. V povezavi z mikrobiološko zbirko je bilo raziskovalno delo osredotočeno na raziskave arktičnih izolatov gliv predvsem iz ledu in sicer na različne rodove nemelaniziranih kvasovk (*Cryptococcus*, *Rhodotorula*, *Leucosporidum*), melaniziranega rodu *Aureobasidium* in pa na filamentozne glive rodu *Penicillium*. Raziskave so obsegale taksonomsko identifikacijo in karakterizacijo teh gliv ter proučevanje njihovih filogenetskih pozicij, fizioloških in morfoloških prilagoditve na pogoje nizke vodne aktivnosti in nizkih temperatur, na produkcije ekstrolitov ter na vlogo, ki jo igrajo v ekologiji polarnih območij.

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

- Krka d.d., Novo mesto; sodelovanje na področju načrtovanja novih zdravilnih učinkovin

ance and fluorescence of green fluorescent proteins strongly depends on the pH. We have prepared improved GFP variant, called RaVe_C, and expressed it in *A.niger.* pKa of RaVe_C is 6.9 which makes it ideal for monitoring cytosolic pH. Characteristics of biosensor in *A.niger* were analyzed using confocal laser microscope and confirmed that expression of RaVe_C was sufficient for visualization and that biosensor responded to the intracellular pH change.

- Within the research of biotechnological use of fungi and their enzymes we have investigated oxidative degradation and decolorization of melanin and synthetic organic dyes and degradation of polyamide-6. In collaboration with our partners abroad we continued our research of proteolytic enzymes for pharmaceutical use, protein hydrolysis and biotransformation of synthetic compounds. In connection with our microbial collection research was focused on isolates of fungi from the arctic environment, predominantly from ice and particularly on different genera of nonmelanized yeasts (*Cryptococcus*, *Rhodotorula*, *Leucosporidum*), melanized *Aureobasidium* and filamentous fungi of *Penicillium*. Research comprised taxonomic identification and characterization of fungi and investigation of their phylogenetic position, physiological and morphological transformation to low water activity and low temperature, production of extrolites and their role in the ecology of the arctic environment.

COLLABORATION WITH INDUSTRY

- Krka d.d., pharmaceutical company, Novo mesto, Slovenia; development and design of bioactive compounds
- Lek d.d., Mengeš, Slovenia; research of fungal metabolism and molecular biology of *Streptomycetes*
- BIA Separations d.o.o., Ljubljana, Slovenia;

- Lek d.d., Mengeš; raziskave na področju metabolizma gliv in molekularne biologije streptomicet,
- BIA Separations d.o.o., Ljubljana; skupni projekt: Afinitetni monolitni nosilci za hitro ločevanje biomolekul

MEDNARODNO SODELOVANJE

v mednarodnih projektih:
- Dva evropska projekta v okviru 5. okvirnega programa: ANTICO in ANEPID
- Bilateralno sodelovanje s Hrvaško, Veliko Britanijo (v okviru programa Partnership in Science (4x)), Portugalsko, Italijo, Madžarsko, Indijo
- COST projekt D25: "Applied biocatalysis: Stereoslective and environmentally-friendly reactions catalysed by enzymes"

pogodbe s podjetji v tujini:
- BASF, Nemčija
- LVMH, Christian Dior Parfums, Francija

z drugimi znanstvenimi ustanovami po svetu:
- Technische Universität Muenchen, Nemčija
- University of Sussex, Velika Britanija
- University of Strathclyde, Glasgow, Škotska
- The University of Edinburgh, Edinburgh, Škotska
- Technical University Denmark, Lyngby, Danska
- Technische Universität Graz, Avstrija
- Agricultural University of Wageningen, Wageningen, Nizozemska
- International Mycological Institute, Egham, Velika Britanija

POMEMBNI INŠTRUMENTI IN DRUGA OPREMA

- UV/VIS spektrofotometer
- Fluorescenčni luminometer PerkinElmer LS-55
- Luminometer / fluorimeter za mikrotitrske plošče z injektorjem

joint project: Affinity monolithic carriers for fast separation of biomolecules

INTERNATIONAL COLLABORATION

International projects:
- Two projects within the 5th Framework Programme: ANTICO and ANEPID
- Bilateral projects with Croatia, Unted Kingdom (within Partnership in Science (4x)), Italy, Hungary, Portugal, India
- Participation at the European Centre of Excellence, contract no. ICA1-CT-2000-70034
- COST project D25: "Applied biocatalysis: Stereoslective and environmentally-friendly reactions catalysed by enzymes"

contracts with companies abroad:
- BASF, Germany
- LVMH, Christian Dior Parfums, France

nonformal collaboration with other research institutions:
- Technische Universität München, Germany
- University of Sussex, UK
- University of Strathclyde, Glasgow, UK
- The University of Edinburgh, Edinburgh, UK
- Technical University Denmark, Lyngby, Denmark
- Technische Universität Graz, Austria
- Agricultural University of Wageningen, Wageningen, Netherlands
- International Mycological Institute, Egham, UK

IMPORTANT INSTRUMENTS AND OTHER EQUIPMENT

- UV/VIS spectrophotometer
- Fluorescence luminometer PerkinElmer LS-55
- Microplate luminometer / fluorimeter with injectors
- Graphical workstation Silicon Graphics Fuel with software for NMR, molecular modeling and SAR analysis

- Grafična postaja Silicon Graphics Fuel s programsko opremo za NMR, molekularno modeliranje in SAR
- Bioreaktorja (Bioengineering, Chemap) Infors
- FIA (flow injection analyser)
- HPLC in drugi kromatografski instrumenti
- Sistem za 2D elektroforezo s programsko opremo (Melanie)
- Laboratorij za delo z mikroorganizmi
- Laboratorij za delo s celičnimi kulturami
- Mikrobiološka zbirka (MZKI)

IZOBRAŽEVALNA DEJAVNOST

- Pet sodelavcev L12 je habilitiranih za sodelovanje pri do- in podiplomskem študiju Univerze v Ljubljani kot predavatelji, dve sodelavki kot asistentki.
- Diplomska dela: 8, magisterij: 1.
- Sodelavci laboratorija so sodelovali pri pripravi tečaja bioinformatike, katerega se je udeležilo več kot 40 biokemikov.
- V L12 se je izobraževalo 8 mladih raziskovalcev.

- Bioreactors (Bioengineering, Chemap) Infors
- FIA (flow injection analyser)
- HPLCs
- System for 2D gel electrophoresis with software for data evaluation (Melanie)
- Laboratories for microbiology and cell culture
- Microbial Culture Collection (MZKI)

EDUCATIONAL ACTIVITY

- Five members of L12 participate as lecturers or demonstrators at the under - and postgraduate level at the University of Ljubljana, Slovenia.
- Eight diploma and one Master's Thesis performed at the department have been defended in 2004.
- Course of Bioinformatics was organized (more than 40 participants).
- Education of 8 young researchers.

L13

Laboratorij za katalizo in reakcijsko inženirstvo

Laboratory for Catalysis and Chemical Reaction Engineering

VODJA / HEAD
Akademik prof. dr. Janez Levec

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

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Matej Komel
Andrej Premrl
Matevž Vospernik
Luka Zevnik

PODROČJA DEJAVNOSTI

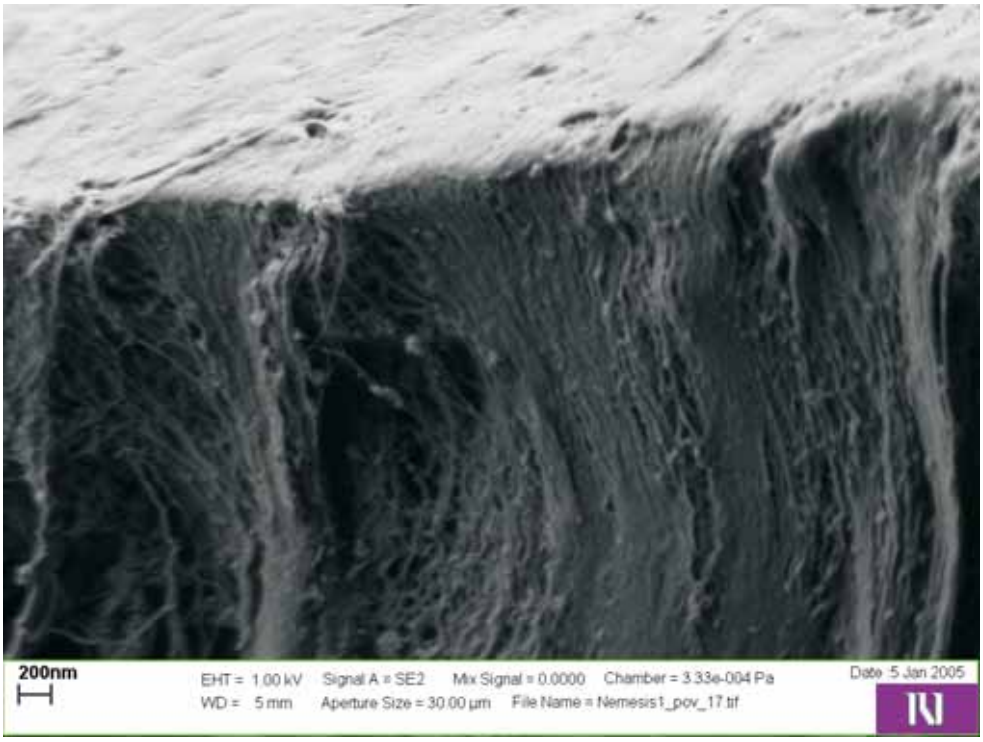
Študij kinetike katalitskih in nekatalitskih reakcij v homogenih in heterogenih reakcijskih sistemih. Priprava katalitsko aktivnih snovi oziroma katalizatorjev. Modeliranje kemijskih reakcij in reaktorjev za enofazne in večfazne reakcije s poudarkom na:

- kinetiki oksidacije vodotopnih organskih onesnaževalcev v trifaznih reaktorjih

RESEARCH ACTIVITIES

Kinetic studies of catalized and non - catalyzed reactions in homogeneous and heterogeneous reaction systems. Preparation of catalytically active compounds and catalysts. Modeling of chemical reactions and reactors for one- and multiphase reactions. In this year the emphasis was given to:

- kinetics of the water - soluble organic pollut-



SLIKA

Dr. Stanko Hočevar (Vodja projekta, Laboratorij za katalizo in reakcijsko inženirstvo) in dr. Andrej Kržan (Laboratorij za polimerno kemijo in tehnologijo) sta v okviru triletnega projekta, ki ga financira Renault, Pariz, Francija, razvila in patentirala nanokompozitno polimerno protonsko prevodno membrano za novo generacijo gorivnih celic (tim. »high-temperature PEMFC«), ki delujejo v temperaturnem območju od 20 do 200°C.

Na sliki je prikazan posnetek prereza membrane pri 300.000 - kratni povečavi z rastrnim elektronskim mikroskopom (operater: dr. Marjan Bele).

FIGURE

Dr. Stanko Hočevar (Project Leader, Laboratory of Catalysis and Chemical Reaction Engineering) and Dr. Andrej Kržan (Laboratory for Polymer Chemistry and Technology) have developed and patented for Renault, Paris, France, a nanocomposite proton conducting membrane for new generation of high - temperature PEM fuel cells, which operates in a temperature window between 20 and 200°C. A three - year project was financed by Renault.

Picture shows a SEM profile of the membrane at 300.000 - fold magnification (Operator: Dr. Marjan Bele).

- interpretaciji eksperimentalnih meritev na osnovi matematičnega modeliranja in optimizacije parametrov
- oksidaciji organskih polutantov v membranskih reaktorjih
- optimizaciji hidrodinamskih pogojev obratovanja eno - in večcevnih membranskih kontaktorjev
- razvoju Pd-Cu in Pd-Sn bimetalnih katalizatorjev, uporabljenih v integriranem procesu za denitrifikacijo podtalnice
- kinetičnih in mehanističnih študijah heterogeno kataliziranih asimetričnih reakcij z in-situ FTIR/ATR metodo
- študiju kinetike in mehanizmov kataliziranih reakcij v procesih proizvodnje in čiščenja vodika ter načrtovanju kompaktnega procesorja za proizvodnjo vodika iz primarnih goriv (fosilnih in obnovljivih) za PEM gorivne celice
- sintezi ter strukturni in elektrokemični karakterizaciji novih anodnih katalizatorjev odpornih na CO za PEM gorivne celice
- sintezi ter strukturni elektrokemični karakterizaciji nanokompozitnih protonsko prevodnih polimernih membran za PEM gorivne celice

BIBLIOGRAFIJA

9 izvirnih znanstvenih člankov
1 drugi članek in sestavek
1 objavljeni znanstveni prispevek na konferenci (vabljeno predavanje)
1 objavljeni znanstveni prispevek na konferenci
8 objavljenih povzetkov znanstvenih prispevkov na konferencah
1 patent
1 predavanje na tuji univerzi
1 končno poročilo o rezultatih raziskav
1 izvedensko mnenje
2 uredništvi revij

ants oxidation in three - phase reactors
- interpretation of experimental data through mathematical modelling and optimization of parameters
- catalytic wet oxidation of organics dissolved in wastewater carried out in membrane reactors
- optimization of process - hydrodynamic conditions in a multi - tube membrane contactor
- development of Pd-Cu and Pd-Sn bimetallic catalysts for integrated process of drinking water denitrification
- kinetic and mechanistic studies of heterogeneously catalyzed asymmetric reactions with in situ FTIR/ATR method
- study of kinetics and mechanisms of catalized reactions in the production and cleaning processes of hydrogen 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

BIBLIOGRAPHY

9 Original Scientific Articles
1 Other Article
1 Published Scientific Conference Contribution (Invited Lecture)
1 Published Scientific Conference Contribution
8 Published Scientific Conference Contribution Abstracts
1 Patent
1 Invited Lecture at Foreign University
1 Final Research Report
1 Expert Opinion
2 Editorships

DOSEŽKI V LETU 2004

- Opredelili smo faktorje, ki kontrolirajo hitrost reakcije v trifaznem membranskem katalitskem reaktorju. Eksperimentalno smo dokazali, da je reakcijska cona zelo ozka in pomaknjena na stran plinastega reaktanta.
- Z analizo rezultatov podzemnega uplinjanja premoga smo ugotovili, da lahko izstopno koncentracijo pri podzemnem uplinjanju premoga napovemo s pomočjo razširjenega termodinamskega modela, ki upošteva vdor vode v izgorevalno votlino, vlažnost premoga in sestavo premoga (CHxOy).
- Določili smo kinetiko reakcije vodnega plina (water gas shift reaction, WGSR) na nanostrukturnem CuxCe1-xO2-y katalizatorju v stacionarnih pogojih.
- V sodelovanju z L07 smo določali elektrokemijske in mehanske lastnosti ter obstojnost nove protonsko prevodne polimerne membrane za visokotemperaturne PEM gorivne celice, ki smo jo razvili in patentirali za Renault, Paris, Francija.
- V sodelovanju z L02 smo določali elektrokemijske in mehanske lastnosti ter obstojnost nove protonsko prevodne polimerne membrane za PEM gorivne celice, ki smo jo razvili v projektu APOLLON (5. OP EU).
- V sodelovanju z L10 smo določali aktivnost in obstojnost novih anodnih katalizatorjev za PEM gorivne celice s povišano odpornostjo proti zastrupljanju s CO, ki smo jih razvili v projektu APOLLON (5. OP EU).

SODELOVANJE Z INDUSTRIJO

Renault, Pariz, Francija; sinteza protonsko prevodnih membran za visokotemperaturne PEM gorivne celice, partnerstvo, projekt po pogodbi (2001 - 2004)

MEDNARODNO SODELOVANJE

- »Waste water treatment by catalytic oxidation contactor« (WATERCATOX), RTD projekt v 5. okvirnem programu EU, pogodba štev. EVK1-CT-2000-00073

RESULTS IN 2004

- Factors controlling the reaction rate in a three - phase membrane catalytic reactor were determined. It was demonstrated experimentally that the reaction zone in the membrane is very thin and shifted towards the gaseous phase reactant.
- Analysis of the underground coal gasification data revealed that the outlet gas composition and concentration can be predicted by means of an expanded thermodynamic model, which takes into consideration the coal composition (CHxOy), its water content and the water outburst into the burning zone.
- Transient kinetic model of CO oxidation over a nanostructured CuxCe1-xO2-y catalyst based on the redox mechanism was developed.
- Determination of electrochemical and mechanical properties and durability of a new proton conducting polymer membrane for high temeprature PEM fuel cell, which was developed and patented in collaboration with L07 within the framework of research project with Renault, Paris, France.
- Determination of electrochemical and mechanical properties and durability of a new proton conducting polymer membrane for PEM fuel cell, which was developed in collaboration with L02 within the framework of APOLLON project (5th FP of EU).
- Determination of activity and durability of a new CO-tolerant anode catalysts for PEM fuel cells in collaboration with L10 in the framework of APOLLON project (5 th FP of EU).

COLLABORATION WITH COMPANIES

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

INTERNATIONAL COLLABORATION

- »Waste water treatment by catalytic oxidation contactor« (WATERCATOX), RTD Project in 5th EU Framework Program, Contract No.:

- »Advanced PEM Fuel Cells« (APOLLON), RTD projekt v 5. okvirnem programu EU, pogodba štev. ENK5-CT-2001-00572

POMEMBNI INŠTRUMENTI IN OPREMA

- računalniško voden tekočinski kromatograf (HP)
- več plinskih kromatografov s TCD in FID detektorjem (HP)
- analizatorja vsebnosti ogljika v tekočih in trdnih vzorcih (Tekman / 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 (Mettler Toledo)
- Automatiziran sistem za karakterizacijo heterogenih katalizatorjev (Micromeritics, model Autochem II 2920)

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA

V okviru sodelovanja v projektu APOLLON (5. OP EU) je dne 18. novembra 2004 Kemijski inštitut obiskal Prof. dr. Jens K. Norskov, direktor Centra za fiziko materialov na atomarni skali Danske tehnične univerze v Lyngbyju (Center for Atomic - Scale Materials Physics, Technical University of Denmark, Lyngby, Danska) in imel predavanje z naslovom "Katalitična in encimatska proizvodnja vodika" (Catalytic and enzymatic hydrogen production).

EVK1-CT-2000-00073

- »Advanced PEM Fuel Cells« (APOLLON), RTD Project in 5 th EU Framework Program, Contract No.: ENK5-CT-2001-00572

IMPORTANT INSTRUMENTS AND EQUIPMENT

- HPLC + ChemStation (HP)
- several GC with TCD and FID detectors (HP)
- TC analyzers in liquid and solid samples (Tekmar / Dohrmann)
- several batch CST, trickle - bed and fixed - bed laboratory reactors with data acquisition and control units
- 600 W fuel cell test station with HP VEE OneLab software - based data acquisition and control unit
- LabMax-ReactIR 1000 reactor and reaction analysis system (Mettler Toledo)
- Automated system for heterogeneous catalysts characterization (Micromeritics, Model Autochem II 2920)

EDUCATION AND IMPORTANT VISITS

Prof. Dr. Jens K. Norskov, Director of the Center for Atomic - Scale Materials Physics, Technical University of Denmark, Lyngby, Denmark, has visited National Institute of Chemistry in the framework of 5th FP EU project APOLLON on 18th November 2004. He delivered a lecture entitled "Catalytic and Enzimatic Hydrogen Production".

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

TEHNIČNO OSEBJE / TECHNICAL STAFF
Špela Božič
Bojan Robič

PRIPRAVNIKI / TRAINEES
Andrej Šonc
Alma Jazbinšek

PODROČJA DEJAVNOSTI

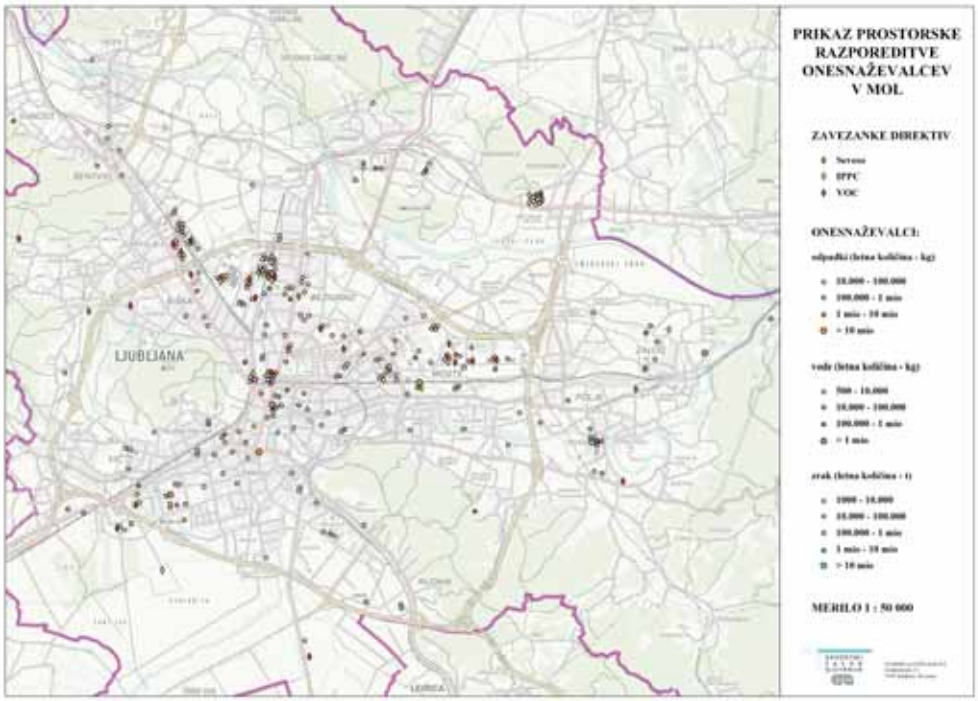
Razvoj procesov

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

RESEARCH ACTIVITIES

Process research and development

- research and development of new industrial products and processes, development of scale - up methods for chemical processes, process simulation and optimization
- measurements of thermodynamic data (e.g. L-V and L-L equilibria) of various industrially important multicomponent liquid mixtures and their modelling by means of statistical thermodynamic methods
- integration of pollution prevention and environmental protection measures for new or existing industrial processes, development of reclamation processes for various components from process waste streams
- development and implementation of methods and procedures for identification, classification and characterization of hazardous



SLIKA

Vpliv industrijskih onesnaževalcev na področju Mestne občine Ljubljana

FIGURE

Impact assessment study of industry on the City of Ljubljana

Čiste tehnologije
- Razvoj in integracija postopkov in preventivnih ukrepov varstva okolja v industrijske procese; uvajanje principov čiste proizvodnje v industrijsko prakso; izdelava ocen skladnosti proizvodnih procesov z BAT tehnologijami po direktivi IPPC
- Razvoj postopkov za regeneracijo uporabnih komponent iz neogibnih odpadnih tokov; zapiranje tehnoloških krogov in uvajanje reciklažnih postopkov; identifikacija, karakterizacija in klasifikacija odpadkov ter razvoj postopkov obdelave in končnega ravnanja z industrijskimi in drugimi odpadki.

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

Servisna dejavnost
- Izvajanje pilotnih poskusov kemijskih sintez in separacij težavnih mešanic večkomponentnih / večfaznih sistemov
- Merjenje izbranih fizikalno - kemijskih lastnosti oz. sestave čistih snovi, mešanic in materialov
- Svetovanje pri izbiri tehnologij ter nakupu, postavitvi in zagonu kemijsko - procesne in okoljevarstvene opreme
- Poskusna proizvodnja specialnih kemičnih izdelkov
- Regeneracija posebno čistih laboratorijskih in procesnih topil.

BIBLIOGRAFIJA

1 izvirni znanstveni članek
3 strokovni članki

wastes; research and development of pretreatment processes for difficult effluents and hazardous wastes
- national environmental balances and inventories of critical contaminants in wastes and emissions; related risk assessment; identification and modelling of transport routes of selected contaminants in the environment

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

BIBLIOGRAPHY

1 Original Scientific Articles
3 Professional Articles
1 Independent Professional Component Part in a Monograph
1 Scientific Article in a Monograph
1 Other Article
4 Published Scientific Conference Contributions
4 Published Professional Conference Contributions
2 Final Research Reports
5 Treatises, Preliminary Studies, Studies
7 Expert Opinions
3 Undergraduate Theses
2 Master's Theses
2 Editorships

RESULTS IN 2004
- Completion of the applied project: Identification of nationally important contaminants of surface waters and preparation of programs for reduction of their negative impacts on the aquatic enviroment. As many as 192 candidate substances were identified as potential polluters, from which the 91 most relevant were identified on the basis of moni-

1 samostojni strokovni sestavek v monografiji
1 samostojni znanstveni sestavek v monografiji
1 drugi članek in sestavek
4 objavljeni znanstveni prispevki na konferencah
4 objavljeni strokovni prispevki na konferencah
2 končni poročili o rezultatih raziskav
5 elaboratov, predštudij, študij
7 izvedenskih mnenj
3 diplome
2 magisterija
2 uredništvi revij

DOSEŽKI V LETU 2004

- Zaključek večletnega projekta: "Identifikacija nevarnih snovi na področju RS in priprava strokovnih podlag za programe zmanjševanja onesnaževanja vodnega okolja z NS" (za MOPE - ARSO): izdelani so kriteriji za izbor nevarnih snovi v okolju, izdelan seznam snovi oz. skupin snovi, ki potencialno najbolj ogrožajo slovenske površinske vode, izdelan seznam dejansko relevantnih snovi, upoštevajoč njihovo porabo v RS in nevarnost za okolje (predvsem strupenost), izdelani osnutki dosjejev relevantnih snovi z emisijskimi in imisijskimi podatki ter predlogi potrebnih ukrepov za zmanjšanje onesnaževanja.
- Izdelava ocene ogroženosti okolja zaradi industrijskega onesnaževanja v Mestni občini Ljubljana, ki obsega najvažnejše sestavine okolja: zrak, vode, odpadke, tla, hrup, rabo surovinskih virov in energentov, industrijska tveganja in celovito preprečevanje onesnaževanja.
- Dogradnja državnega informacijskega sistema in izdelava nacionalnih bilanc komunalnih, nenevarnih in nevarnih odpadkov za leto 2003, s časovno vrsto od leta 1999, po dejavnostih in kataloških vrstah odpadkov.
- Izdelava nacionalne bilance emisij hlapnih organskih snovi iz industrije, določitev ukrepov za dosego predpisanega zmanjšanja toring data in all environmental media and trade data. The preliminary pollution reduction programmes were prepared for all which has enough data to evaluate, for others asurveilance monitoring was proposed in order to provide the data. Programmes take into account the available toxicity data, up - to - now measures, substance national inventories, and emission - immission monitoring records.
- Environmental impact assessment study of the Ljubljana metropolitan basin. The main industrial pollution sources were identified with respect to their emissions into the air, surface waters, waste generation, noise, resource conservation and energy efficiency, chemicals and industrial hazards, response to various directives (IPPC, VOC, Seveso) etc. Spatial distribution of sources and threads was presented and some prevention measures proposed.
- National information system on waste generation: upgrade of the data collection system and update of databases for municipal, industrial and hazardous wastes, generated during the years 2002 - 2003 in various sectors according to NACE classification and EWC; time trends were shown for the period since 1999.
- National inventory and information system on the industrial emission of volatile organic compounds, distribution of emissions between industrial sectors, measures identification for reduction of the excess emissions, cost estimation, prediction of emission reduction by implementing various measures till 2020.
- Completion of the project "Cleaner Production 2003 / 2004", aiming the introduction of UNEP -based methodology for a proactive environmental management system into selected Slovene companies. In the one year programme nine companies were participting, which accomplished large savings and emission reduction.
- Participation in the Centre of Exellence (coordinator Jozef Stefan Institute, Ljubljana,

emisij, ocena stroškov, ocena poteka emisij do leta 2020.

- Vzpostava sodelovanja z Univerzo Erlangen, Nemčija na področju razvoja in modeliranja sproščanja zdravilnih učinkovin.
- Koordiniranje, soizvajanje in dokončanje projekta "Čista proizvodnja 2003 / 2004" za uvajanje metodologije Cleaner Production v izbrana slovenska podjetja. V letni program je bilo vključenih devet večjih in srednjih podjetij, ki so uspešno upeljala ta prostovoljni sistem ravnanja z okoljem in na vzorčnih primerih izkazala 182 mio SIT prihrankov, ob tem pa tudi velika zmanjšanja emisij v okolje.
- Izdelava sistemske dokumentacije in upeljevanje sistema za zagotavljanje kvalitete preskusov karakterizacije odpadkov po standardu SIST EN ISO 17025 v naš laboratorij.
- Vključitev v center odličnosti Ekološke tehnologije (nosilec IJS), sofinanciran iz strukturnih skladov EU, s programom razvijanja čiste tehnologije predelave tehnične fosforne kisline v čisto kislino oz. njene soli z uporabo nove generacije ekstraktantov.
- Delo v okviru slovenskega tekstilnega grozda na programih vzpostavljanja ekološke komponente trajnostnega razvoja varstva okolja v tekstilni industriji (preprečevanje onesnaževanja, ločevanje in recikliranje odpadkov, čiščenje in recikliranje odpadnih vod, obdelava emisij v zrak).
- Sodelovanje s procesno - tehničnim oddelkom Univerze v Erlangenu, Nemčija na razvoju novih tehnik in nosilcev za kontrolirano sproščanje zdravilnih učinkovin.
- Pridobitev poblastila za okoljsko izvedenstvo po Zakonu o varstvu okolja (Ad personam - vodja laboratorija) in za presojo okoljskega ravnanja podjetij po sistemu EMAS (v sodelovanju s SIQ).

SODELOVANJE Z INDUSTRIJO

- TKI Hrastnik d.d., Hrastnik
- Belinka - Perkemija d.o.o., Ljubljana

Slovenia), co - funded by EU - SFD, with R&D project on clean technology development in the field of pure phosphoric acid / salts production, by using an integrated extraction - adsorption - desorption process.

- Participation in the R&D programme of the slovene textile cluster, aiming towards introduction of sustainable development measures into textile industry processes (emission prevention, waste minimisation / recycling).
- Starting the collaboration with University of Erlangen, Germany, on drug release processes modelling and development (three months stay of a research fellow).

COLLABORATION WITH COMPANIES

- Pilot - plant experiments, process modelling and optimization (non-catalytic chemical syntheses, component / phase separation, mixing etc.)
- waste identification, analysis and classification
- waste prevention and minimisation
- consulting in process optimisation, equipment selection and environmental protection
- small scale production of specialty chemicals, recovery of extra pure solvents from waste mixtures
- environmental impact assessment studies

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 200 litres), semibatch and continuous mode of operation; supported by corresponding infrastructure, measuring / control equipment, personal and process computers & software
- Equipment for measurement and modelling of thermodynamic equilibrium of various

- Lek d.d., Ljubljana
- Liveo d.o.o., Ljubljana
- MOPE - ARSO, Ljubljana

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 200 litrov; s pripadajočo infrastrukturo, merilno - regulacijsko opremo, računalniško programsko opremo za načrtovanje procesov ter analizo in obdelavo podatkov
- Oprema za določanje in modeliranje faznih ravnotežij tekočina - para, tekočina - tekočina in tekočina - trdno za potrebe načrtovanja separacijskih procesov npr. destilacije, rektifikacije, ekstrakcije, absorpcije, adsorpcije, sušenja, kristalizacije ipd.
- Programska oprema za modeliranje in vodenje procesov (ASPEN+, FIX, PARAGON, PROCEDE ...)

IZOBRAŽEVANJE

Mentorstva:

- 2 magistrski deli
- 3 diplomska dela

Habilitacije:

- V. Grilc: izr. prof., kemijsko inženirstvo (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani); poučevanje: Gospodarjenje z odpadnimi snovmi (Univerza v Ljubljani, Fakulteta za gradbeništvo in geodezijo - Vodarstvo in komunalno inženirstvo), Ravnanje z odpadki (Interfakultetni podiplomski študij varstva okolja, Univerza v Ljubljani), MBA Studies in Sustainable industrial development - Clean Technology Management, ICPE, Ljubljana
- L. Fele Žilnik: znanstvena sodelavka, kemijsko inženirstvo (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani), poučevanje: gostujoča predavateljica za del predmeta Termodifuzijske operacije (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani).

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

Supervison of student projects:

- 2 MSc project
- 3 BSc projects

Assignments:

- V. Grilc: assistant professor in chemical engineering
- L. Fele Žilnik: research fellow in chemical engineering

(both at Univerity of Ljubljana, Faculty for Chemistry and Chemical Technology)

L15

Nacionalni center za NMR spektroskopijo visoke ločljivosti - lokacija KI

National Centre for High Resolution NMR Spectroscopy - Location NIC

VODJA / HEAD
Doc. dr. Janez Plavec

RAZISKOVALCI / RESEARCHERS
Dr. Matjaž Polak
Dr. Martin Črnugelj
Dr. Simona Golič Grdadolnik (delno / partly)
Dr. Gregor Mali (delno / partly)
Dr. Iztok Jože Košir (delno / partly)

MLADI RAZISKOVALCI / YOUNG RESEARCHERS
Miha Plevnik
Primož Šket
Mirko Cevec

TEHNIČNO OSEBJE / TECHNICAL STAFF
Aleksandar Gaćeša
Damjan Makuc

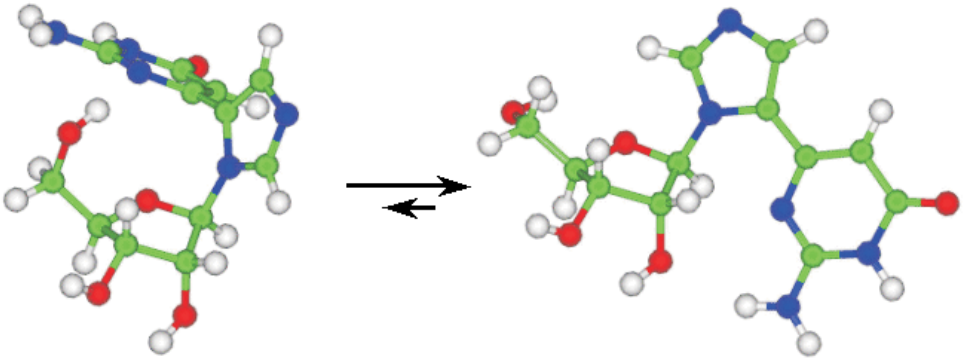
PODROČJA DEJAVNOSTI

V program delovanja NMR centra za leto 2004 so bile vključene NMR meritve in raziskave za vse uporabnike, ki so le te potrebovali in uporabljali pri svojem raziskovalnem in razvojnem delu v okviru osnovnih in aplikativnih raziskav in projektov za industrijo ali v industriji sami. NMR centre upravlja Programski svet v sestavi: prof. dr. Robert Blinc (Institut Jožef Stefan, Ljubljana - predsednik), dr. Darko Kocjan (Lek d.d., Ljubljana - namestnik predsednika), dr. Janez Smodiš (Krka d.d., Novo mesto), prof. dr. Venčeslav Kaučič (KI), dr. Jurka Kidrič (KI), prof. dr. Dani Kikelj (Fakulteta za farmacijo Univerze v Ljubljani), dr. Mitja Kocjančič (Kmetijski inštitut Slovenije), prof. dr. Branko Stanovnik (Fakulteta za kemijo in kemijsko tehnologijo Univerze v Ljubljani), dr. Zoran Šušterič (Sava d.d., Kranj) in dr. Miloš Komac (MVŠZT).

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 2004 included NMR measurements and research for academic institutions and researchers from industrial partners. Research program of NMR centre includes data acquisition and interpretation for those who apply NMR in their research as part of basic and applied research projects or in industry itself. Annual research program was discussed and approved by the Scientific council of NMR centre.

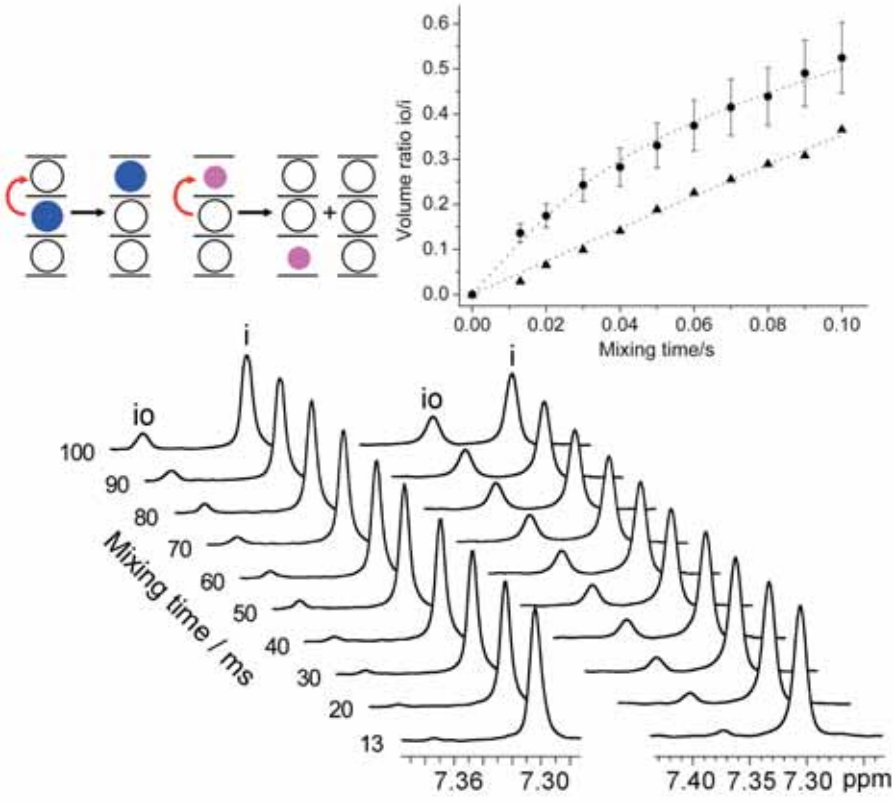


SLIKA 1

V članku z naslovom "Conformational Properties of Shape Modified Nucleosides - Fleximers", ki je bil objavljen v reviji J. Am. Chem. Soc. (2004, 126, 8159) so M. Polak, K. L. Seley in J. Plavec objavili detajlno 1H NMR konformacijsko študijo fleksimirnih nukleozidov v primerjavi z njihovimi naravnimi analogi, ki so jo dopolnili z ab initio izračuni. Sprememba purinske nukleinske baze v naravnih nukleozidih z bolj fleksibilno bazo močno poveča populacijo anti konformer okoli glikozidne vezi. To je povezano s pomikom pseudorotacijskega ravnotežja k konformeram Severnega tipa, ki ni bil pričakovan glede na povečano sterično oviranost nukleinske baze.

FIGURE 1

In the manuscript entitled "Conformational Properties of Shape Modified Nucleosides - Fleximers" published in J. Am. Chem. Soc. (2004, 126, 8159) M. Polak, K. L. Seley and J. Plavec have described detailed 1H NMR conformational study complemented with ab initio computations on fleximer nucleosides in relation to their natural counterparts in solution. The change of purine nucleobase in natural nucleosides with more flexible nucleobase strongly increases the populations of anti conformation around glycosyl bond. This was accompanied with a large shift towards North-type sugar conformation that was not expected upon indicated increase of steric bulk of nucleobase.



SLIKA 2

V članku z naslovom "$^{15}NH_4^+$ ion movement inside $d(G_4T_4G_4)_2$ G-quadruplex is accelerated in the presence of smaller Na^+ ions", ki je bil objavljen v reviji Org. Biomol. Chem. (2004, 2, 1970) so P. Šket, M. Črnugelj, W. Kozminski in J. Plavec demonstrirali, da je izmenjava amonijevih ionov med različnimi vezavnimi mesti med pari gvaninskih kvartetov 7.5-krat hitrejša v prisotnosti natrijevih ionov. Spektri na sliki predstavljajo sledi vzdolž f2 v 2D ^{15}N-1H NzExHSQC spectrih pri kemijskem premiku ^{15}N 29.5 ppm v odvisnosti od mešalnega časa, ki je podan v sliki na levi. Spektri na levi ustrezajo vzorcu $d(G_4T_4G_4)_2$ kvadrupleksa zvitega v prisotnosti 20 mM $^{15}NH_4Cl$, medtem ko tisti na desni ustrezajo vzorcu istega G-kvadrupleksa v prisotnosti 20 mM $^{15}NH_4Cl$ in 5 mM NaCl. Graf odvisnosti volumskih razmerij kot funkcija mešalnega časa smo uporabili za izračun hitrostne konstante amonijevega iona med notranjim in zunanjim vezanim mestom (slika na desni zgoraj).

FIGURE 2

In the manuscript entitled "$^{15}NH_4^+$ ion movement inside $d(G_4T_4G_4)_2$ G-quadruplex is accelerated in the presence of smaller Na+ ions" published in Org. Biomol. Chem. (2004, 2, 1970) P. Šket, M. Črnugelj, W. Kozminski and J. Plavec have demonstrated that ammonium ion movement between different binding sites sandwiched by two guanine-quartets is accelerated by 7.5 times in the presence of sodium ions. Spectra in the figure represent traces along f2 dimension of 2D ^{15}N-1H NzExHSQC spectrum at ^{15}N of 29.5 ppm as a function of increasing mixing time given in ms on the left. Stack of spectra on the left correspond to $d(G_4T_4G_4)_2$ sample folded in the presence of 20 mM $^{15}NH_4Cl$, whereas the set on the right corresponds to the same G-quadruplex in the presence of 20 mM $^{15}NH_4Cl$ and 5 mM NaCl. Plots of volume ratios as a function of mixing time were used to calculate rate constants for the ammonium ion movement from the inner to the outer binding site (figure on the top right).

Program dela NMR centra za leto 2004 je obravnaval in potrdil Programski svet NMR centra. V letu 2004 je delo NMR centra potekalo v okviru 78 programov in projektov. Raziskave v okviru NMR centra so v letu 2004 izvajali raziskovalci naslednjih domačih institucij, ki so soustanoviteljice in sovlagateljice v nakup instrumentov NMR centra: Kemijskega inštituta Ljubljana, Instituta Jožef Stefan Ljubljana, Fakultete za farmacijo in Fakultete za kemijo in kemijsko tehnologijo Univerze v Ljubljani. V zadnjih nekaj letih smo sodelovanje NMR centra na Kemijskem inštitutu razširili na uporabnike iz NUKa, Biotehniške in Medicinske fakultete Univerze v Ljubljani. Instrumenti so na razpolago vsem ustanovam in podjetjem, ki jih potrebujejo pri svojem delu. Podjetja Lek d.d., Ljubljana; Krka d.d., Novo mesto in Helios d.d., Domžale jih kot sovlagatelji pri nakupu osnovne opreme NMR centra uporabljajo pri rutinski analitiki in v okviru svojega raziskovalno - razvojnega dela. V letu 2004 so instrumente v okviru NMR centra na KI uporabljali tudi raziskovalci iz podjetij Fenolit d.d., Borovnica; Pliva, Zagreb, Hrvaška in Donau Chemie, Brückl, Nemčija.

Raziskave v NMR centru so obsegale:

- študij strukture oligomernih fragmentov nukleinskih kislin ter konformacijskih sprememb gradnikov DNK ob interakciji s kovinskimi ioni
- študij strukture in dinamike proteinov, intermediatov pri zvitju proteinov in molekularnih interakcij peptidov z lipopolisaharidi
- študij strukture in dinamike antibiotikov v povezavi z njihovim biološkim učinkom
- študij interakcij antibiotikov kot je n.pr. vankomicin z membranami
- raziskave strukture in dinamike organskih molekul, detekcija in karakterizacija reaktivnih intermediatov pri reakcijah organskih in organokovinskih spojin
- študij naravnih produktov
- študij sprememb v eritrocitih med bolezenskimi stanji

Current members of the scientific council are: Prof. Dr. Robert Blinc (Jozef Stefan Institute, Ljubljana, Slovenia - president) and Prof. Dr. Branko Stanovnik (Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia), Prof. Dr. Venčeslav Kaučič (NIC), Dr. Jurka Kidrič (NIC), Prof. Dr. Daniel Kikelj (Faculty of Pharmacy, University of Ljubljana, Slovenia), Dr. Janez Smodiš (Krka d.d., Novo mesto, Slovenia), Dr. Darko Kocjan (Lek d.d., Ljubljana, Slovenia), Dr. Zoran Šušterič (Sava d.d., Kranj, Slovenia), Dr. Mitja Kocjančič (Agricultural Institute of Slovenia) and Dr. Miloš Komac (Ministry of Higher Education, Science and Technology of the Republic of Slovenia).

In 2004 the cooperation between various research groups and NMR centre at NIC involved 78 basic, applied and industrial projects as well as international research projects. Research was conducted by the following academic institutions that are cofounders and coinvestors into equipment of NMR centre: National Institute of Chemistry, Institute Jozef Stefan, Faculty of Chemistry and Chemical Technology and Faculty of Farmacy. In the last few years cooperation of NMR centre at NIC has been extended to colleagues at National University Library, Faculty of Biotechnolgy and Medicinal Faculty. Instruments are available to all institutions and companies which apply NMR spectroscopy at their work. Companies Lek, Krka and Helios use NMR spectrometers as analytical tool as well as in their research and development projects. In 2004 NMR centre offered services and help to companies Fenolit, Pliva in Donau Chemie.

Research activities of NMR centre are focused on:

- studies on structure of oligomeric DNA fragments and conformational changes in DNA building blocks upon interaction with metal ions
- studies of protein structure and dynamics, protein folding intermediates and molecular interactions of peptides with lipopolysaharides

- študij strukture in konformacijskih ravnotežij metabolitov v raztopini in v trdnem
- določanje neželenih stranskih in razgradnih produktov v zdravilih
- karakterizacijo kemijskih struktur poroznih materialov na fosfatni osnovi in strukturnih sprememb v procesu hidrotermalne sinteze zeolitov
- študij strukture in čistosti polimernih materialov, vsebnosti stranskih produktov polimerizacije, mehanizmov polimerizacije, lastnosti polimerov z načrtovano makromolekularno strukturo
- določanje kvalitete ter geografskega porekla slovenskih vin

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

NMR centru je EU v okviru 5. okvirnega programa podelila naziv Center odličnosti EU. Projekt Centra odličnosti v NMR centru na KI je tekel od 1. novembra 2000 do 31. oktobra 2004. Projekt Centra odličnosti je sestavljalo enajst delovnih paketov, ki so jih vodili odgovorni nosilci s KI.

Leto 2004 je pomembno zaznamovalo dogajanje okoli posodobitve opreme NMR centra z investicijo v nov 800 MHz NMR spektrometer in obnovo obstoječe opreme. Investicijo je Programski svet NMR centra podprl že leta 2001. Spomladi 2004 smo skupaj s sodelavci iz podjetij Lek d.d., Ljubljana in Krka d.d., Novo mesto pripravili ambiciozen projekt Centra odličnosti z naslovom "NMR centre odličnosti za študij struktur in interakcij v biotehnologiji in farmaciji". Raziskovalno - razvojne usmeritve so zajete v 5 podsklopih oz. delovnih paketih, s katerimi fokusiramo naše aktivnosti na naslednja znanstvena in raziskovalna vprašanja, ki se zelo tesno navezujejo na konkretne probleme v farmacevtski industriji:

- studies on structure and dynamics of antibiotics in relation with their biological role
- studies on interactions of antibiotics such as vancomycin with membranes
- structure and dynamics of organic molecules, detection and characterization of reactive intermediates in reactions of organic and organometallic compounds
- studies on natural products
- studies on changes in erythrocytes during disease
- structure and conformational equilibria of metabolites in solution and in solid state,
- determination of by products in pharmaceuticals
- structural characterization of phosphate based porous materials and structural changes in the process of hydrothermal synthesis of zeolites
- studies on structure and purity of polymeres, 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.

NMR centre has been awarded title Centre of Excellence by EU. Activities within Centre of Excellence project run since November 1st 2000 and project finished on October 31st 2004. Project consisted of eleven work packages which were led by principal investigators from NIC.

The major activities in 2004 involved upgrade of equipment of NMR centre which includes investment into a new 800 MHz NMR spectrometer and upgrade of existing equipment. Proposal was supported by Scientific council of

1. Struktura in interakcije v trdnem stanju, polikristaliničnost, polimorfizem
2. Struktura in analitika organskih spojin v raztopini
3. Raziskave zmesi spojin v raztopini - profil nečistoč v zdravilih, razpadni produkti, metaboliti
4. Karakterizacija rekombinantnih proteinov in bioloških makromolekul v raztopini
5. Interakcija zdravilnih učinkovin z biološkimi makromolekulami

BIBLIOGRAFIJA

11 izvirnih znanstvenih člankov
2 objavljena znanstvena prispevka na konferencah
3 objavljeni povzetki znanstvenih prispevkov na konferencah
1 objavljeni povzetek strokovnega prispevka na konferenci
1 prispevek na konferenci brez natisa
1 projektna dokumentacija
1 diploma

GLAVNI DOSEŽKI V LETU 2004

- Projekt Centra odličnosti, ki smo ga skupaj pripravili sodelavci Kemijskega inštituta, Leka in Krke je bil izbran v financiranje.
- Izvedli smo razpis za nov 800 MHz in posodobitev že obstoječih NMR spektrometrov. Istočasno so potekale aktivnosti za gradnjo novega objekta, v katerem bo nameščen nov NMR spektrometer.
- Raziskovalni dosežki, ki so nastali v sodelovanju NMR centra z raziskovalnimi laboratoriji in skupinami širom po Sloveniji so bili objavljeni v preko 33 publikacijah v revijah z mednarodnim recenzentskim sistemom (seznam je dostopen na domači strani NMR centra na naslovu: http://www.nmr.ki.si). Precejšnje število teh dosežkov je bilo objavljenih v revijah, ki segajo v sam vrh znotraj posameznih področij znanosti. Ti dosežki bodo posebej opisani med rezultati

NMR centre already in 2001. In Spring 2004 we and researchers from Lek d.d., Ljubljana, Slovenia and Krka d.d., Novo mesto, Slovenia prepared and submitted ambitious proposal of Centre of Excellence entitled "NMR centre of excellence for the study of structures and interactions in biotechnology and pharmacy". Research and development orientations are divided into 5 sub-areas or work-packages. These areas are tightly linked to problems in the pharmaceutical industry and will allow us to focus our activities on the following scientific and research questions:

1. Structure and interactions in solid state, polycrystallinity, polymorphism
2. Structural determination and analysis of organic compounds in solution
3. Studies of mixtures of compounds in solution - profiling of impurities in medicines, degradation products, metabolites
4. Characterization of recombinant proteins and biological macromolecules in solution
5. Interaction of medically active compounds with biological macromolecules

BIBLIOGRAPHY

11 Original Scientific Articles
2 Published Scientific Conference Contributions
3 Published Scientific Conference Contribution Abstracts
1 Published Professional Conference Contribution Abstract
1 Unpublished Conference Contribution
1 Project Documentation
1 Undergraduate Thesis

IMPORTANT ACHIEVEMENTS IN 2004

- Project Centre of Excellence prepared jointly by researchers from NIC, Lek d.d., Ljubljana, Slovenia and Krka d.d., Novo mesto, Slovenia has been approved.
- Tender for a new 800 MHz and upgrade of existing NMR spectrometers has been realized. At the same time activities for construct-

posameznih laboratorijev Kemijskega inštituta ali na drugih inštitutih in fakultetah. Dosežki sodelovanja med NMR centrom in slovensko industrijo so javno znani le preko uspešnega poslovnega rezultata posameznega podjetja. Na tem mestu bi posebej omenili le en dosežek raziskovalne skupine dr. Janeza Plavca, ki se ukvarja s študijem strukture in konformacijskih ravnotežij nukleozidov, nukleotidov in oligomernih fragmentov nukleinskih kislin v raztopini z uporabo eno in večdimenzionalnih NMR metod. V letu 2004 smo dokončali konformacijsko študijo modificiranih nukleozidov, v katerih sta imidazolski in pirimidinski del obroča v purinskem skeletu ločena z enojno vezjo (t.i. fleksimeri). Rezultati te študije so bili objavljeni pod naslovom "Conformational Properties of Shape Modified Nucleosides - Fleximers" v prestižni periodiki J. Am. Chem. Soc. (2004, 126, 8159).

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

NMR centre je infrastrukturni centre, ki nudi podporo najširšemu krogu akademskih in ostalih uporabnikov. Zelo intenzivni so stiki z industrijskimi partnerji, ki so sovlagatelji v opremo NMR centra:

- Krka tovarna zdravil d.d., Novo mesto
- Lek farmacevtska družba d.d., Ljubljana
- Helios d.d., Domžale

Ostali uporabniki uslug NMR centra so v letu 2004 bili:

- Fenolit d.d., Borovnica
- Pliva, Zagreb, Hrvaška
- Donau Chemie, Brückl, Nemčija

MEDNARODNO SODELOVANJE

Mednarodno sodelovanje NMR centra je obsežno. EU komisija je NMR centre v okviru 5. okvirnega programa izbrala za Center odličnosti EU s projektom: "Use of NMR Spectroscopy in Combination with Computational Methods on

ing a new building for new NMR spectrometer were moving ahead.

- Scientific achievements, which are the result of cooperation of NMR centre with laboratories and groups around Slovenia were published in over 33 publications in journals with international peer review evaluation procedure (complete list is available on NMR centre's home - page at http://www.nmr.ki.si). Several of these publications were published in journals which are at the top of the list within individual scientific fields. These achievements will be specifically described as results of individual laboratories at NIC or other institutes or faculties. Results of cooperation between NMR centre and Slovenian industry are publicly known only through positive financial results of individual company. One achievement of the group of Dr. Janez Plavec, which is involved in studies and conformational equilibira of nucleosides, nucleotides and oligomeric fragments of nucleic acids in solution with the use of one and multidimensional NMR methods is mentioned here. In 2004 we have completed conformational study of modified nucleosides, in which imidazole and pyrimidine moieties of purine ring are split but remain connected by a single bond (i.e. fleximers). Results of the study were published in an article entitled "Conformational Properties of Shape Modified Nucleosides - Fleximers" in prestigious periodical J. Am. Chem. Soc. (2004, 126, 8159).

COLLABORATION WITH INDUSTRIAL AND OTHER PARTNERS

NMR centre 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 are co-owners of the equipment and regular users of NMR facility:

- Krka d.d., Novo mesto, Slovenia

Systems of Biological Interest". Projekt se je leta 2004 zaključil.
Med skupino dr. Plavca in prof. dr. Nicholasa Huda, Georgia Institute of Technology, Atlanta, ZDA poteka dolgoletno sodelovanje. Trenutno je financirano v okviru NATO Science Programme CLG projekta z naslovom "Solution State Investigations of DNA Quadruplex Structure and Cation Binding".

POMEMBNI INŠTRUMENTI IN OPREMA
V okviru NMR centra na lokaciji KI so nameščeni sledeči NMR spektrometri visoke ločljivosti:
- Varian Unity Inova 600
- Varian Unity Inova 300
- Varian Unity plus 300

IZOBRAŽEVANJE IN OBISKI / GOSTOVANJA
Pomemben vidik delovanja NMR centra je njegova izobraževalna vloga. NMR centre nudi pomoč pri snemanju in interpretaciji NMR spektrov pri konkretnih strukturnih problemih v okviru diplomskih del, magisterijev in doktoratov.
V skupini vodje NMR centra je leta 2004 svoje dodiplomsko izobraževanje zaključil Gregor Ilc z diplomskih delom z naslovom "Vpliv modifikacij na gvaninskem obroču na tvorbo G-kvadrupleksov".

- Lek d.d., Ljubljana, Slovenia
- Helios d.d., Domžale, Slovenia

The other users of our services and expertise in 2004 were:
- Fenolit d.d., Borovnica, Slovenia
- Pliva, Zagreb, Croatia
- Donau Chemie, Brückl, Germany

INTERNATIONAL COLLABORATION
NMR centre is very active internationally. Slovenian NMR centre was selected and nominated by European Commission as Centre of Excellence with the project: "Use of NMR Spectroscopy in Combination with Computational Methods on Systems of Biological Interest". The project has come to a successful completion in 2004.
Collaboration between the groups of Professors Janez Plavec and Nicholas Hud, Georgia Institute of Technology, Atlanta, USA has been continuing for several years. At the moment it is financed through NATO Science Programme CLG project entitled "Solution State Investigations of DNA Quadruplex Structure and Cation Binding".

MAJOR EQUIPMENT
Major equipment of NMR centre includes high-resolution NMR spectrometers:
- Varian Unity Inova 600
- Varian Unity Inova 300
- Varian Unity Plus 300

EDUCATION AND IMPORTANT VISITS
Important aspect of NMR centre 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.
Mr. Gregor Ilc has successfully completed his undergraduate education in the group of the head of NMR centre by diploma thesis entitled "The role of modifications on guanine residue on the formation of G-quadruplexes".

L16

Center za validacijske tehnologije in analitiko (CVTA)

Center 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 / associates from L06:
Dr. Mirko Prošek L6 (vodja področja / Head of program)
Dr. Alenka Golc Wondra (vodja področja / Head of program)
Mitja Križman, univ. dipl. kem.

TEHNIČNO OSEBJE / TECHNICAL STAFF
Ana Andrić, kem. tehn.
Mag. Nadja Gerčar, univ. dipl. inž. kem. tehn. (do / until 28. 2. 2004)
Katarina Jankovič, inž. tekst. tehn.
Adolf Krašna, univ. dipl. inž. kem. tehn.
Darija Lorber, inž. kem. tehn.
Tanja Maver, univ. dipl. inž. živil. tehn.
Katja Rožmanc Babnik, univ. dipl. inž. kem. tehn.
Barbara Lečnik Spaić, univ. dipl. kem. (od / since 1. 11. 2004)

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
- načtrovanje in izvedbo validacij analiznih postopkov

ACTIVITIES IN 2004

CVTA designs and performs the folowing activities related to medicines and food:

- development of HPLC, GC, TLC and other analytical procedures
- analyses and analytical studies for quality control of products, and validation of production and cleaning technologies

SLIKA 1
Priprava vzorcev za vrednotenje farmacevtske tehnologije

FIGURE 1
Samples preparation for evaluation of a pharmaceutical technology

- izvajanje analiz in analiznih študij za potrebe kontrole kakovosti izdelkov ter validacij proizvodnih tehnologij in tehnologij čiščenja proizvodne opreme
- izvajanje bioanaliznih za študij biorazpoložljivosti oz. bioekvivalentnosti zdravil
- validacije analiznih metod in tehnologij z navedenimi tehnikami
- izdelavo ekspertnih mnenj in svetovanja na področju dejavnosti

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

- bioanylitical 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 2004

CVTA was established as a unit of the institute in the year 2002 to follow the increasing needs of pharmaceutical industry for analytical sup-

SLIKA 2
Priprava vzorcev za vrednotenje farmacevtske tehnologije

FIGURE 2
Samples preparation for evaluation of a pharmaceutical technology

GLAVNI DOSEŽKI V LETU 2004

CVTA je bil kot samostojna organizacijska enota ustanovljen v letu 2002 zaradi naraščajočih potreb slovenske farmacevtske industrije po analitski podpori razvojnim in proizvodnim projektom ob zaostrovanju kakovostnih zahtev za izvajanje takšnih del. V osnovi predstavlja novi model izvajanja nalog za potrebe industrije, ki smo ga v l. 2004 nadalje uspešno razvijali ter organizacijsko in vsebinsko prilagajali potrebam naročnikov. Tako smo v redno delo po zahtevah dobre laboratorijske oz. dobre proizvodne prakse uvedli plinsko kromatografijo, dejavnost pa smo razširili na nove tipe nalog, kot so stabilitetne študije in kontrola kakovosti končnih farmacevstkih izdelkov. Proti koncu leta smo začeli tudi z uvajanjem testiranja hitrosti raztapljanja učinkovin (disolucij); tehniko bomo uvedli v l. 2005. Delo v CVTA poteka ob strokovni podpori Laboratorija za prehrambeno kemijo (L06).

V l. 2004 smo za slovensko farmacevtsko industrijo izvedli:

- razvoj štirih analitskih postopkov
- 1 bioanalitsko študijo (na ca 60 prostovoljcih)
- validacijo 66 HPLC, GC in TLC analitskih postopkov
- analize za validacijo več proizvodnih tehnologij
- analize za validacije več tehnologij čiščenja proizvodne opreme
- analize v okviru stabilitetnih študij za več preparatov
- analize rezidualnih topil v ca. 500 vzorcih

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

SODELOVANJE Z INDUSTRIJSKIMI IN DRUGIMI PARTNERJI

V skladu s cilji ustanovitve je CVTA vse prihodke v l. 2004 ustvaril z delom za domačo farmacevtsko industrijo, zlasti z družbama Lek d.d., Ljubljana in Krka d.d., Novo mesto.

port to their R&D and production projects, combined with sharpening requirements of quality standards. In principle it represents a novel organizational model, which was in 2004 successfully further developed and adjusted to the needs of industrial partners. In this respect we have introduced gas chromatography into current work under the GLP and GMP standards, as well as some new types of work, such as stability studies and quality control of finished dosages forms. Towards end of the year we have also started to add dissolution testing to the portfolio of CVTA techniques. All the activities were performed in tight collaboration with L06, which offered professional support of its experts to CVTA.

Crucial achievements in the year 2004 are:

- Development of 4 analytical methods
- 1 bioanalytical study (approximately 60 volunteers included)
- Validation of 66 HPLC, GC in TLC analytical methods
- Analyses for several process validations
- Analyses afor several cleaning validations
- Analyses for stability studies
- Analyses of residual solvents (OVI) in approximately 500 samples

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

MAJOR EQUIPMENT

Several HPLC systems, two GC and TLC system, all validated and operating according to GLP principles.

POMEMBNI INŠTRUMENTI IN OPREMA

Več HPLC sistemov, dva GC sistema in TLC sistem (skupaj z L06). Vsi instrumenti so validirani in delujejo v skladu s principi dobre laboratorijske prakse (GLP).

Zaposleni v splošnem sektorju

General Sector - Employees

UPRAVA / ADMINISTRATION
Izidor Babnik
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RAČUNOVODSTVO IN KOMERCIALA / ACCOUNTING AND PROCUREMENT
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Boštjan Genorio
Tadej Smerkolj
David Šarlah
Kljačič Alen

L01

Laboratorij za molekularno modeliranje in NMR spektroskopijo

Laboratory for Molecular Modelling and NMR Spectroscopy

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

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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L02

Laboratorij za spektroskopijo materialov

Laboratory for Spectroscopy of Materials

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

1. DUBČEK, Pavo, TURKOVIĆ, Aleksandra, CRNJAK OREL, Zorica, ETLINGER, Božidar, BERNSTORFF, Sigrid. Synchrotron light scattering on nanostructured V/Ce oxide films intercalated with Li^+ ions. *J. Chem. Inf. Comput. Sci.*, 2004, vol. 44, no. 2, str. 290-295. [COBISS.SI-ID 3004186]

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L03

Laboratorij za kemometrijo

Laboratory of Chemometrics

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

1. BALABAN, Alexandru T., RANDIĆ, Milan. Partitioning of pi-electrons in rings of polycyclic conjugated hydrocarbons. 5, Nonalternant compounds. *J. Chem. Inf. Comput. Sci.*, 2004, vol. 44, no. 5, str. 1701-1707. [COBISS.SI-ID 3183130]

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9. MLINŠEK, Gregor, NOVIČ, Marjana, KOTNIK, Miha, ŠOLMAJER, Tomaž. Enzyme binding selectivity prediction : α-thrombin vs trypsin inhibition. *J. Chem. Inf. Comput. Sci.*, 2004, vol. 44, no. 5, str. 1872-1882. [COBISS.SI-ID 3085338]

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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Mentorstva / Mentorships

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Uredništva / Editorships

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L04

Laboratorij za analizno kemijo

Laboratory for Analytical Chemistry

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

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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Doktorati, magisteriji in diplome / Ph.D., M.Sc. and B.Sc. Theses

23. KOVAČEVIČ, Miroslav, Veber, Marjan (mentor), Novič, Milko (komentor). Application of hyphenated system liquid chromatography - element mass spectrometry for characterisation of organophosphorus compounds = Uporaba sklopljenega sistema tekočinska kromatografija - elementna masna spektrometrija za karakterizacijo organofosfornih spojin : doctoral dissertation = doktorsko delo. Ljubljana: [M. Kovačevič], 2004. VIII, 101 f., ilustr., tabele. [COBISS.SI-ID 3001626]

24. PODKRAJŠEK, Boštjan, Grgić, Irena (mentor), Veber, Marjan (komentor). Vpliv mangana in karboksilnih kislin na oksidacijo žveplovih(IV) zvrsti v troposferski vodni fazi : doktorska disertacija. Ljubljana: [B. Podkrajšek], 2004. II, 102 f., ilustr. [COBISS.SI-ID 3164186]

Mentorstva / Mentorships

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Članstva v organizacijskih odborih / Memberships in Conference Committees

27. CERJAN-STEFANOVIĆ, Štefica, NOVIČ, Milko. Members of organizing committee. 7th ISIC - International school of IC : Motovun, 29.9. - 02.10.2004. Motovun [Croatia], 29.sep.-2.okt.2004. [COBISS.SI-ID 3127578]

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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. COTMAN, Magda, ZAGORC-KONČAN, Jana, ŽGAJNAR GOTVAJN, Andreja. The relationship between composition and toxicity of tannery wastewater. *Water Sci. Technol.*, 2004, vol. 49, no. 1, str. 39-46, graf. prikazi. [COBISS.SI-ID 25665285]

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

8. DROBNE, Damjana, JEMEC, Anita, SEPČIĆ, Kristina, SIMČIČ, Tatjana, BRANCELJ, Anton, MILANI, Marziale, ZRIMEC, Alexis, DRINOVEC, Luka, KOSTANJŠEK, Rok, ŠTRUS, Jasna. Visualization of oxygen radical-dependent photoemission from digestive glands of isopods (Crustacea) after exposure to chemical stress. V: BERDEN ZRIMEC, Maja (ur.), ZRIMEC, Alexis (ur.), DROBNE, Damjana (ur.), MILANI, Marziale (ur.). Weak photon emission from living tissues : delayed luminescence - facts & perspectives. 1st ed. Grosuplje: Institute for Physical Biology, 2004, str. 64-65. [COBISS.SI-ID 1423951]

9. ROŠ, Milenko. Čiščenje komunalnih odpadnih vod v Sloveniji. V: ROŠ, Milenko (ur.). [Simpozij] Vodni dnevi 2004, Velenje, 7.-8. oktober 2004. Zbornik referatov. Ljubljana: Slovensko društvo za zaščito voda: = Slovenian Water Pollution Control Association: = Slowenische Vereinigung für Gewässerschutz, 2004, str. 1-5. [COBISS.SI-ID 3124762]

10. ROŠ, Milenko. Onesnaževanje slovenskih vodotokov : [vabljeno predavanje]. V: OTRIN, Andrej (ur.), PORENTA, Marijan (ur.). Posvetovanje Vodni zadrževalniki – razvojna nuja ali nedopustni posegi v naravo. Zbornik referatov. Ljubljana: Elektrotehniška zveza Slovenije, 2004, str. 27-36, graf. prikazi. [COBISS.SI-ID 3152666]

11. TOMAŽEVIČ, Erna, ROŠ, Milenko. Emisije hraniv iz komunalnih bioloških čistilnih naprav : vabljeno predavanje. V: ROŠ, Milenko (ur.). [Simpozij] Vodni dnevi 2004, Velenje, 7.-8. oktober 2004. Zbornik referatov. Ljubljana: Slovensko društvo za zaščito voda: = Slovenian Water Pollution Control Association: = Slowenische Vereinigung für Gewässerschutz, 2004, str. 6-13. [COBISS.SI-ID 3125018]

12. GRILC, Viktor, ROŠ, Milenko, ŽITKO ŠTEMBERGER, Nataša. Programi za zmanjševanje onesnaževanja slovenskega vodnega okolja z nevarnimi snovmi = Preparation of pollution prevention programmes for Slovene surface water environment. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). Jubilejni 10. Slovenski kemijski dnevi 2004, Maribor, 23. in 24. september 2004. Maribor: FKKT, 2004, str. [1-8] (Abstrakt v Zborniku referatov s posvetovanja, str. 41). [COBISS.SI-ID 3116570]

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Monografije in sestavki v monografijah / Monographs and Contributions in Monographs

16. DROLC, Andreja, ROŠ, Milenko. Assuring comparability of results of nitrate determinations in wastewater : application of metrological principles. V: POPOV, Viktor (ur.). Second International conference on waste management, Rhodes, Greece, 29 September-1 October 2004. Waste management and the environment. II. Southampton; Boston: Wit Press, cop. 2004, str. [595]-604. [COBISS.SI-ID 3106074]

17. ROŠ, Milenko. Modern small wastewater treatment plants. V: NOVAK-PINTARIČ, Zorka (ur.), SIMONIČ, Marjana (ur.), IRŠIČ BEDENIK, Nataša (ur.). Environmental protection. Maribor: ŠOUM, 2004, str. 77-87. [COBISS.SI-ID 3073562]

18. ZUPANČIČ, Gregor Drago. Biological sludge management. V: NOVAK-PINTARIČ, Zorka (ur.), SIMONIČ, Marjana (ur.), IRŠIČ BEDENIK, Nataša (ur.). Environmental protection. Maribor: ŠOUM, 2004, str. 88-99. [COBISS.SI-ID 3073818]

Doktorati, magisteriji in diplome / Ph.D., M.Sc. and B.Sc. Theses

19. COTMAN, Magda, Zagorc-Končan, Jana (mentor). Razvoj nove strategije za oceno vplivov ekotoksikoloških potencialov odpadne vode na reko : doktorska disertacija. Ljubljana: [M. Cotman], 2004. XIII, 139 f., ilustr. [COBISS.SI-ID 26015237]

Mentorstva / Mentorships

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L06

Laboratorij za prehrambeno kemijo in Center za validacijske tehnologije in analitiko (CVTA)

Laboratory for Food Chemistry and Centre for Validation Technologies and Analytics (CVTA)

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

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L07

Laboratorij za polimerno kemijo in tehnologijo

Laboratory for Polymer Chemistry and Technology

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

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

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19. ANŽLOVAR, Alojz, ŽIGON, Majda. Prepletene polimerne mreže na osnovi funkcionaliziranih poliuretanov in poliakrilatov = Interpenetrating polymer networks on the basis of functionalized polyurethanes and polyacrylates. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). Jubilejni 10. Slovenski kemijski dnevi 2004, Maribor, 23. in 24. september 2004. Maribor: FKKT, 2004, str. [1-10] (Abstrakt v Zborniku referatov s posvetovanja, str. 58). [COBISS.SI-ID 3115802]

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Patenti in patentne prijave / Patents and Patent Applications

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Mentorstva / Mentorships

27. ČULIN, Jelena, Veksli, Zorica (mentor), Žigon, Majda, Anžlovar Alojz (delovna mentorja za področje sinteze). Fazno razdvajanje i molekulska dinamika u djelomice interpenetriranim mrežama na temelju poliuretana i polimetakrilata = Phase separation and molecular dynamics of semi-interpenetrated networks based on polyurethanes and polymethacrylates : dizertacija = dissertation. Zagreb: Prirodoslovno-matematički fakultet Sveučilišta u Zagrebu, Kemijski odsjek, 2004. IV, 101 f., V, ilustr. [COBISS.SI-ID 3201818]

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Članstva v organizacijskih odborih / Memberships in Conference Committees

29. GANDINI, Alessandro, SANADI, Anand, KRŽAN, Andrej, CAULFIELD, Daniel F., CHIELLINI, Emo, GALEMBECK, Fernando, CARDENAS, Galo, BRAUNEGG, Gerhart, CHODÁK, Ivan, SAINTE BEUVE, Jérôme, KURUVILLA, Joseph, REBOREDO, María Marta, DURÁN, Nelson, EL SEOUD, Omar Abdel, NARAYAN, Ramani, MIERTUS, Stanislav, HEINZE, Thomas. Members of the International Advisory Committee. 5th International Symposium on Natural Polymers and Composites [also ISNaPol] & 8th Brazilian Symposium on the Chemistry of Lignins and other Wood Components. Sao Pedro [SP, Brazil], 12-15 September, 2004. [COBISS.SI-ID 3176474]

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Uredništva / Editorships

31. Materiali in tehnologije. Žigon, Majda (področni urednik 2000-). Ljubljana: Inštitut za kovinske materiale in tehnologije, 2000-. ISSN 1580-2949. [COBISS.SI-ID 106193664]

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L08

Laboratorij za organsko sintezo in kemijo zdravil

Laboratory for Organic and Medicinal Chemistry

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

1. JAKŠA, Suzana, KRALJ, Bogdan, PANNECOUQUE, Christophe, BALZARINI, Jan, DE CLERCQ, Erik, KOBE, Jože. How a modification (8-aza-3-deaza-2'-deoxyguanosine) influences the quadruplex structure of Hotoda's 6-mer TGGGAG with 5'- and 3'-end modifications. *Nucleos. Nucleot. & Nucleic Acids*, 2004, vol. 23, no. 1/2, str. 77-88. [COBISS.SI-ID 2933786]

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3. KALAYANOV, Genadiy, JAKŠA, Suzana, SCARCIA, Tommaso, KOBE, Jože. Regioselective functionalization of guanine : simple and practical synthesis of 7- and 9-alkylated guanines starting from guanosine. *Synthesis (Stuttg.)*, 2004, vol. 11, no. 12, str. 2026-2034. [COBISS.SI-ID 3078938]

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8. STEPHAN, Michel, MOHAR, Barbara. Préparation de l'acide 6-hydroxycaproique et d'autres ω-hydroxycarboxyliques monomériques de haute pureté = Preparation of highly pure monomeric 6-hydroxycaproic acid and other ω-hydroxycarboxylic acids : brevet d'invention BR0604A/01, la date de la demande 21 juin 2004. Paris: INPI - Institute nationale de la proprieté industrielle, 2004. [COBISS.SI-ID 3077146]

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Uredništva / Editorships

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L09

Laboratorij za anorgansko kemijo in tehnologijo

Laboratory for Inorganic Chemistry and Technology

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

1. KOSANOVIĆ, Cleo, SUBOTIĆ, Boris, KRANJC, Edi. Kinetic analysis of isothermal crystallization of low-carnegieite from precipitated amorphous aluminosilicate precursor. *Micropor. Mesopor. Mat.*, 2004, vol. 71, no. 1/3, str. 27-32. [COBISS.SI-ID 3052314]

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V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

8. GABROVŠEK, Roman, KAUČIČ, Venčeslav. Nanoporoznost in obstojnost betonov visokih zmogljivosti. V: ZAJC, Andrej (ur.). Gradnja z betoni visokih zmogljivosti : zbornik gradiv in referatov. Ljubljana: IRMA, Inštitut za raziskavo materialov in aplikacije, 2004, str. [67]-69. [COBISS.SI-ID 3050266]

9. KAUČIČ, Venčeslav. Nanoporous materials : [invited lecture]. V: 4th International conference of the chemical societies of the South-East European countries [also] ICOSECS 4 on chemical sciences in changing times : visions, challenges and solutions : book of abstracts. Vol. 2. Belgrade: Serbian Chemical Society, 2004, str. 8. [COBISS.SI-ID 3079706]

10. HORVAT, Andrej, KAUČIČ, Venčeslav, GOLOB, Janvit. Razpršilno sušenje topnih silikatov = Spray drying of soluble silicates. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). Jubilejni 10. Slovenski kemijski dnevi 2004, Maribor, 23. in 24. september 2004. Maribor: FKKT, 2004, str. [1-8] (Abstrakt v Zborniku referatov s posvetovanja, str. 138). [COBISS.SI-ID 3113242]

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13. HORVAT, Andrej, Golob, Janvit (mentor), Kaučič, Venčeslav (komentor), Knez, Željko (član komisije za zagovor). Tehnike sušenja izbranih silikatov do proizvodov s specifičnimi fizikalno-kemijskimi lastnostmi : doktorska disertacija. Ljubljana: [A. Horvat], 2004. XIII, 119 f., ilustr. [COBISS.SI-ID 26323205]

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16. International journal of molecular sciences. Kaučič, Venčeslav (član uredniškega odbora 2001-). Basel: MDPI Center. ISSN 1422-0067. [COBISS.SI-ID 2779162]

17. Microporous and mesoporous materials. Kaučič, Venčeslav (član uredniškega odbora 2003-). Amsterdam (etc.): Elsevier, 1998-. ISSN 1387-1811. [COBISS.SI-ID 1595162]

L10

Laboratorij za elektrokemijo materialov

Laboratory for Materials Electrochemistry

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

1. ARČON, Denis, ZORKO, Andrej, CEVC, Pavel, DOMINKO, Robert, BELE, Marjan, JAMNIK, Janko, JAGLIČIĆ, Zvonko, GOLOSOVSKY, I. Weak ferromagnetism of $LiMnPO_4$. *J. Phys. Chem. Solids. [Print ed.]*, 2004, vol. 65, str. 1773-1777. [COBISS.SI-ID 18511143]

2. ARČON, Denis, ZORKO, Andrej, DOMINKO, Robert, JAGLIČIĆ, Zvonko. A comparative study of magnetic propertis of $LiFePO_4$ and $LiMnPO_4$. *J. Phys., Condens. Matter.*, 2004, vol. 16, str. 5531-5548. [COBISS.SI-ID 18328103]

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5. SEVER ŠKAPIN, Andrijana, GABERŠČEK, Miran, DOMINKO, Robert, BELE, Marjan, DROFENIK, Jernej, JAMNIK, Janko. Detection of highly conductive pathways in $LiMn_2O_4$-carbon black composites for Li ion batteries by microcontact impedance spectroscopy. *Solid State Ion. [Print ed.]*, 2004, vol. 167, no. 3/4, str. 229-235. [COBISS.SI-ID 3023898]

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7. VRBANIĆ, Daniel, REMŠKAR, Maja, JESIH, Adolf, MRZEL, Aleš, UMEK, Polona, PONIKVAR, Maja, JANČAR, Boštjan, MEDEN, Anton, NOVOSEL, Barbara, PEJOVNIK, Stane, VENTURINI, Peter, COLEMAN, J. C., MIHAILOVIĆ, Dragan. Air-stable monodispersed $Mo_6S_3I_6$ nanowires. *Nanotechnol. (Bristol)*, 2004, vol. 15, str. 635-638. [COBISS.SI-ID 18208807]

8. DOMINKO, Robert. Nove kompozitne elektrode za litijeve ionske akumulatorje. *Novice - IJS (Tisk. izd.)*, apr. 2004, št. 111, str. 19-22, ilustr. [COBISS.SI-ID 3024154]

9. VENTURINI, Peter. Na znanju temelječa družba potrebuje znanje!. V: Pogovori o prihodnosti Slovenije. Pogovor 3, O vlogi znanja in znanosti : Ljubljana, 10. december 2003. Ljubljana: Urad Predsednika Republike Slovenije, 2004, str. 191-193. [COBISS.SI-ID 3147034]

V celoti objavljeni prispevki s konferenc / Full Text Conference Contributions

10. PEJOVNIK, Stane, BELE, Marjan, GABERŠČEK, Miran, DOMINKO, Robert, DROFENIK, Jernej, JAMNIK, Janko. Gelatin-modified surfaces in selected electronic components. V: NAIR, K. M. (ur.), BHALLA, Amar (ur.), HIRANO, Shin'ichi (ur.), SUVOROV, Danilo (ur.), ZHU, W. (ur.), SCHWARTZ, R. (ur.). Ceramic materials and multilayer electronic devices : proceedings of the High Strain Piezoelectric Materials, Devices, and Applications and Advanced Dielectric Materials and Multilayer Electronic Devices Symposia : held at the 105th Annual Meeting of the American Ceramic Society : April 27-30, 2003 in Nashville, Tennessee, (Ceramic transactions, v. 150). Westerville: American Ceramic Society, cop. 2004, str. 417-426. [COBISS.SI-ID 3092250]

11. BELE, Marjan, DMITRAŠINOVIĆ, Djordje, PLANINŠEK, Odon, SALOBIR, Mateja, SRČIČ, Stanko, GABERŠČEK, Miran, JAMNIK, Janko. Kontrolirano sproščanje zdravilnih učinkovin : klaritromicin, prevlečen s silicijevim dioksidom = Controlled release of drugs : silica coatings on clarithromycin. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). Jubilejni 10. Slovenski kemijski dnevi 2004, Maribor, 23. in 24. september 2004. Maribor: FKKT, 2004, str. [1-7] (Abstrakt v Zborniku referatov s posvetovanja, str. 40). [COBISS.SI-ID 3115290]

12. DOMINKO, Robert, BELE, Marjan, GABERŠČEK, Miran, REMŠKAR, Maja, HANŽEL, Darko, JAMNIK, Janko. Porous olivin composites synthesized by sol-gel technique : [poster]. V: BESENHARD, Jürgen Otto (ur.). Battery and fuel cell materials : extended abstracts of the Battery and fuel cell materials symposium, Graz (Austria), April 18-22, 2004. Graz: International Battery Materials Association, 2004, str. 125-126 (no. 62). [COBISS.SI-ID 3027738]

13. GABERŠČEK, Miran, DOMINKO, Robert, BELE, Marjan, PEJOVNIK, Stane, REMŠKAR, Maja, HANŽEL, Darko, JAMNIK, Janko. Polprevodniški katodni materiali za litijeve ionske akumulatorje : ali mikroporoznost lahko nadomesti nano delce? = Semiconducting cathode materials for lithium ion rechargeable batteries : can microporosity replace nano particles? : [poster]. V: GLAVIČ, Peter (ur.), BRODNJAK-VONČINA, Darinka (ur.). Jubilejni 10. Slovenski kemijski dnevi 2004, Maribor, 23. in 24. september 2004. Maribor: FKKT, 2004, str. [1-6] (Abstrakt v Zborniku referatov s posvetovanja, str. 101). [COBISS.SI-ID 3116826]

14. GABERŠČEK, Miran, DOMINKO, Robert, BELE, Marjan, REMŠKAR, Maja, HANŽEL, Darko, JAMNIK, Janko. Nanoporous, carbon-painted lithium storage materials : [lecture]. V: GOJO, Miroslav (ur.). 3. hrvatski simpozij o elektrokemiji = 3rd Croation symposium on electrochemistry, Dubrovnik, 30.5-3.6.2004. Zbornik radova. Zagreb: Hrvatsko društvo kemijskih inženjera i tehnologa, 2004, str. 97-100. [COBISS.SI-ID 3188762]

15. SEVER ŠKAPIN, Andrijana, GABERŠČEK, Miran, DOMINKO, Robert, BELE, Marjan, JAMNIK, Janko. Use of microcontact impedance spectroscopy in characterization of modern battery materials. V: GOJO, Miroslav (ur.). 3. hrvatski simpozij o elektrokemiji = 3rd Croation symposium on electrochemistry, Dubrovnik, 30.5-3.6.2004. Zbornik radova. Zagreb: Hrvatsko društvo kemijskih inženjera i tehnologa, 2004, str. 85-88. [COBISS.SI-ID 990055]

16. TURKOVIĆ, Aleksandra, GABERŠČEK, Miran. Impedance spectroscopy of nanostructured TiO_2 films on glass substrate as electrode for dye-sensitized solar cell : [lecture]. V: GOJO, Miroslav (ur.). 3. hrvatski simpozij o elektrokemiji = 3rd Croation symposium on electrochemistry, Dubrovnik, 30.5-3.6.2004. Zbornik radova. Zagreb: Hrvatsko društvo kemijskih inženjera i tehnologa, 2004, str. 101-104. [COBISS.SI-ID 3189018]

17. VRBANIĆ, Daniel, MEDEN, Anton, JANČAR, Boštjan, PONIKVAR, Maja, NOVOSEL, Barbara, VENTURINI, Peter, PEJOVNIK, Stane, MIHAILOVIĆ, Dragan. $Mo_6S_3I_6$ nanowires. V: KUZMANY, Hans (ur.). Electronic properties of synthetic nanostructures : XVIII International Winterschool/ Euroconference on Electronic Properties of Novel Materials, Kirchberg, Tirol, Austria, 6-13 March 2004, (AIP conference proceedings, v. 723). Melville: American Institute of Physics, 2004, str. 423-426. [COBISS.SI-ID 18599975]

Mentorstva / Mentorships

18. DMITRAŠINOVIĆ, Djordje, Srčič, Stanko (mentor), Gaberšček, Miran (komentor). Priprava kompozitov SiO_2-klaritromicin za prirejeno sproščanje = Preparation of SiO_2-clarythromycin composites for controlled release : diplomska naloga, (Fakulteta za farmacijo, Ljubljana, Diplomske naloge, 1870). Ljubljana: [Dmitrašinović, Dj.], 2004. 58 f., ilustr. [COBISS.SI-ID 1479281]

19. GRGIĆ, Krešimir, Planinšek, Odon (mentor), Bele, Marjan (komentor). Vpliv pomožnih snovi na raztapljanje naproksena po obarjanju iz zmesi topil = The influence of additives on dissolution of naproxen after the precipitation from mixture of solvents : diplomska naloga, (Fakulteta za farmacijo, Ljubljana, Diplomske naloge, 1894). Ljubljana: [Grgić, K.], 2004. 52 f., ilustr. [COBISS.SI-ID 1536369]MONOGRAFIJE IN DRUGA ZAKLJUČENA DELA

Patenti in patentne prijave / Patents and Patent Applications

20. BELE, Marjan, DOMINKO, Robert, GABERŠČEK, Miran, JAMNIK, Janko. Postopek priprave katodnega materiala v litijevih akumulatorjih, material katode in katoda : patent št. 21529, datum objave 31.12.2004 : po prijavi št. 200300135, datum prijave 4.6.2003. Ljubljana: Urad Republike Slovenije za intelektualno lastnino, 2003/2004. [COBISS.SI-ID 2893338]

Članstva v organizacijskih odborih / Memberships in Conference Committees

21. JENKO, Monika, LAMUT, Jakob, PREŠERN, Vasilij, LAGOJA, Aleš, VODOPIVEC, Franc, GREŠOVNIK, Ferdinand, VENTURINI, Peter, PEJOVNIK, Stane, DROFENIK, Mihael, KOBE, Spomenka, SUVOROV, Danilo, KOSEC, Marija, ŽIGON, Majda, GASPERIČ, Jože, LEGAT, Andraž, STEINER PETROVIČ, Darja, TORKAR, Matjaž, HUSKIĆ, Miroslav, PREGELJ, Andrej, GRABKE, Hans Jürgen, PETZOW, Günter, MILUN, Milorad, DUŠEK, Karel. Člani znanstvenega/organizacijskega/mednarodnega znanstvenega odbora = Members of scientific/organizing/international scientific committee. 12. konferenca o materialih in tehnologijah = 12th Conference on Materials and Technology. Portorož, Slovenia, 27-29 September 2004. [COBISS.SI-ID 3197978]

22. MAIER, Joachim, SCHOONMAN, Johannes, RIESS, Ilan, KROK, Franciszek, MOLENDA, Janina, JAMNIK, Janko, GABERŠČEK, Miran, BELE, Marjan, DOMINKO, Robert, STRMČNIK, Dušan, ZORKO, Milena. Members of programme committee and members of local organizing committee. 7th ISSFIT - International symposium on systems with fast ionic transport. Bled (Slovenia): National Institute of Chemistry, 2004. [COBISS.SI-ID 3024666]

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Uredništva / Editorships

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L11

Laboratorij za biosintezo in biotransformacijo

Laboratory for Biosynthesis and Biotransformation

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

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Uredništva / Editorships

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L12

Laboratorij za biotehnologijo

Laboratory of Biotechnology

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

1. ANDRÄ, Jörg, GARIDEL, Patrick, MAJERLE, Andreja, JERALA, Roman, RIDGE, Richard, PAUS, Erik, NOVITSKY, Tom, KOCH, Michel H. J., BRANDENBURG, Klaus. Biophysical characterization of the interaction of Limulus polyphemus endotoxin neutralizing protein with lipopolysaccharide. *Eur. J. Biochem.*, 2004, vol. 271, no. 10, str. 2037-2046. [COBISS.SI-ID 3021594]

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Mentorstva / Mentorships

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L13

Laboratorij za katalizo in reakcijsko inženirstvo

Laboratory for Catalysis and Chemical Reaction Engineering

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L14

Laboratorij za procesno inženirstvo

Laboratory for Chemical Process Engineering

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L15

Nacionalni center za NMR spektroskopijo visoke ločljivosti - lokacija KI

National Centre for High Resolution NMR Spectroscopy - Location NIC

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

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