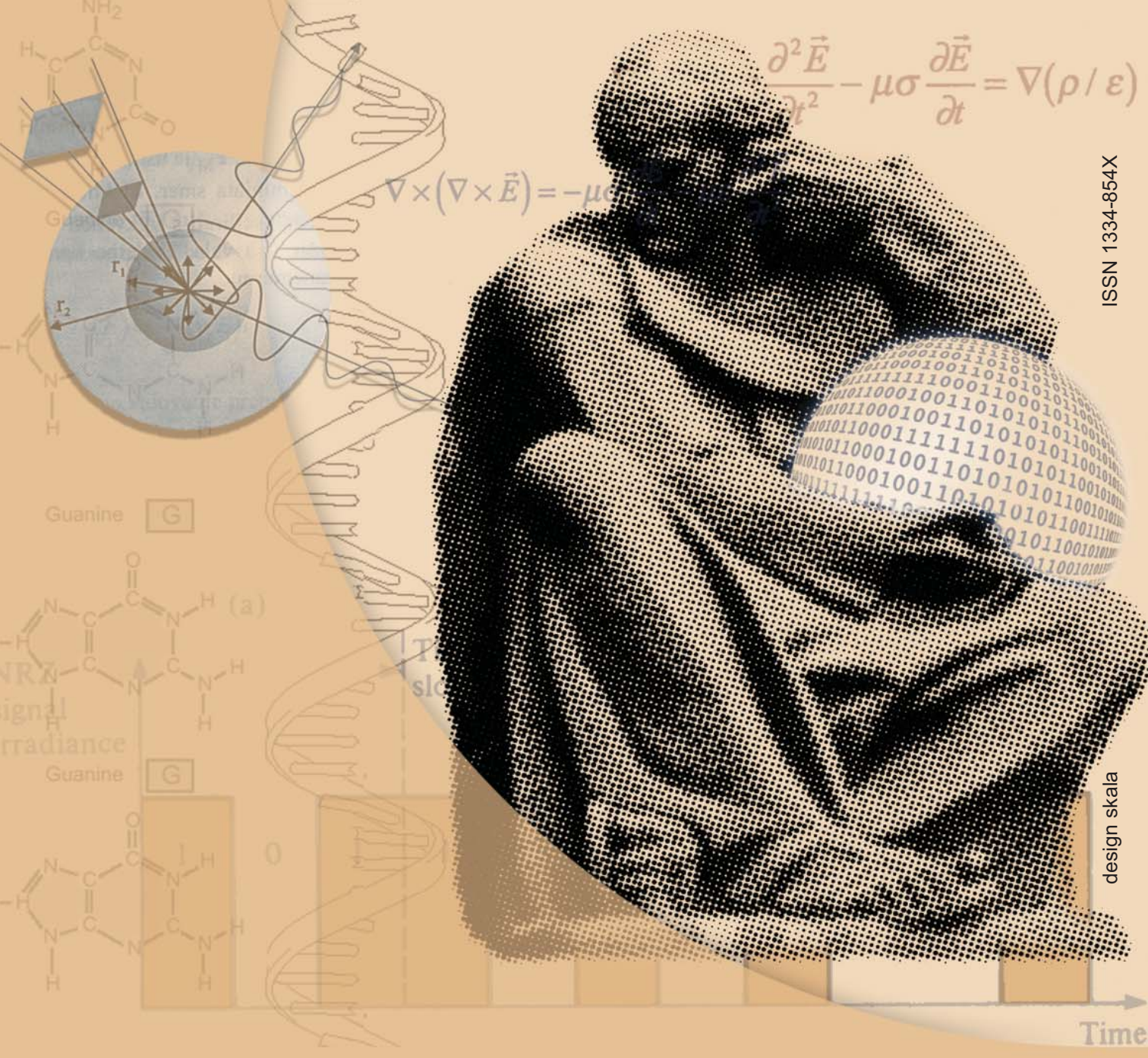

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Ruđer Bošković Institute

Annual Report 2004

Ruđer Bošković Institute

Annual Report 2004

Arial view of the RBI campus

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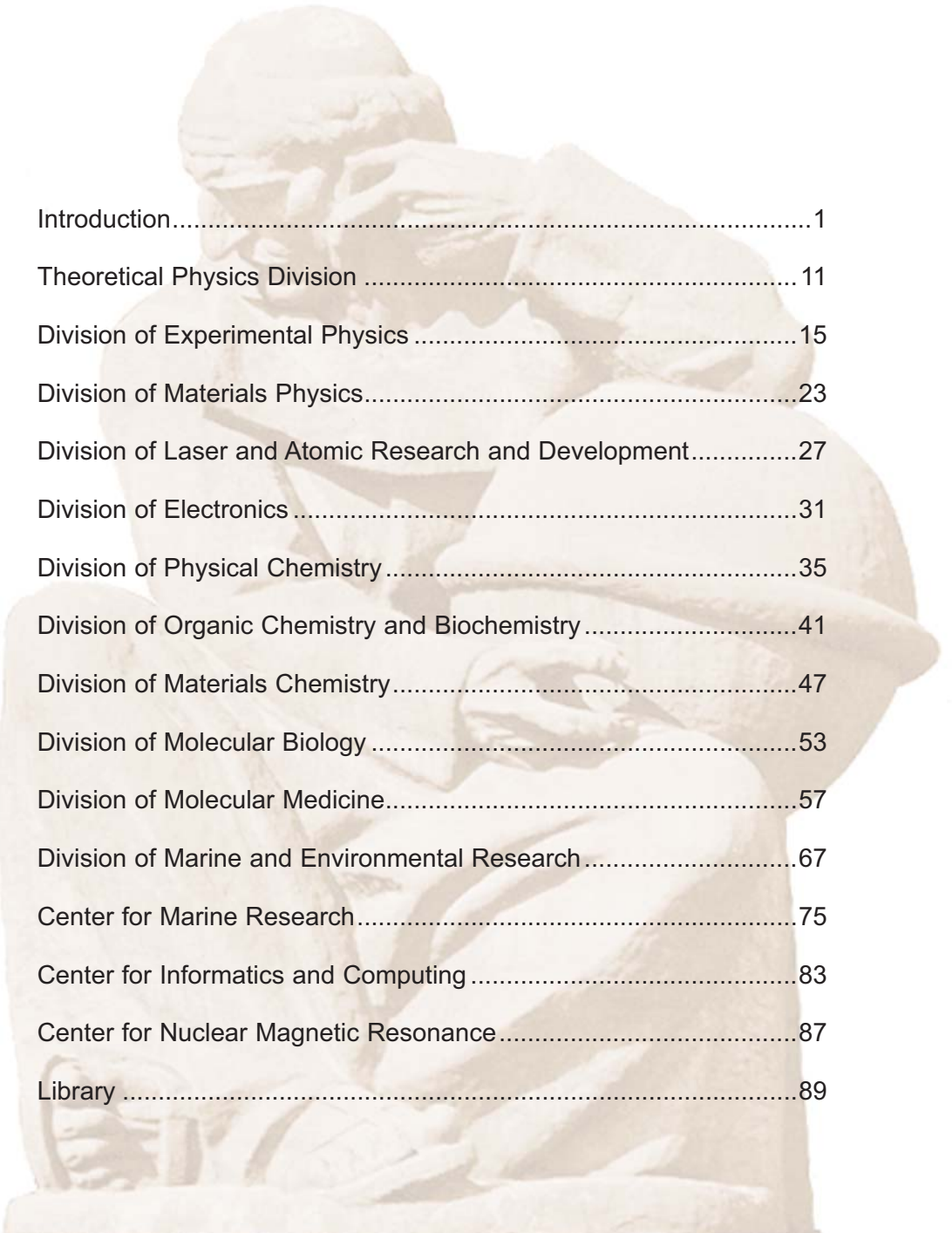


Introduction

INTRODUCTION

Even a brief perusal of the following pages describing the results, achievements and discoveries during 2004 instils a sense of pride in the progress of scientific work at the Ruđer Bošković Institute (RBI). We find there experimental and theoretical works on the properties of the smallest constituents of matter or studies of the structures on vast cosmological scales. New materials were found and characterised, some of interest in electronics, others in medical applications. New stable or long-lived molecules were synthesized and novel enzymes were isolated and characterised. Atmospheric ozone data, marine gel phases, alien jellyfish, algae, or pollutants in the Adriatic were followed and analysed. In medical research, a new inherited disease was identified and characterised at the genetic level while several important advances in tumour regulating genes, suppressors or signalling pathways were discovered and described.

As our scientific work continues to excel, developments outside of RBI indicate approaching changes. On June 18, 2004, the Brussels European Council accepted Croatia as a candidate country. Whether it will be during 2008 or another year, Croatia is becoming a part of the European Research Area and the Institute needs to adjust its policies and standards to the level of the EU.

The ascension of Croatia to the EU will be very positive for RBI but more ominous changes are apparent on both the national and global level. Nationally, the budgetary policy of continually increasing debt is unsustainable and the science and higher education sectors are being asked to contribute towards an adjustment. Globally, in the longer term of two or three decades, a critical shortage of crude oil and climate change based on the current levels of carbon dioxide in the atmosphere are inevitable. Carbon emission restrictions will be far more stringent than those of the Kyoto protocol. The world is accepting these facts, and during 2004 the price of uranium more than doubled. All these changes will bring important future responsibilities for the nuclear and environmental scientists at RBI.

The Institute recognizes the need for monitoring and improving its performance in all aspects of its mission. During 2004, numerous discussions were held on the nature of the mission, the future directions and the governing structure of RBI. Many of the debates were initiated as a result of the World Bank Science and Technology Project (STP) that included a blueprint for reform of RBI.

The Institute did not dispute the need for improved commercial performance but was of the opinion that, after very long and exten-

sive consultations, the chief problem is the inadequacy of the current national legislative and regulatory framework, of which the most notable deficiencies are the mandatory promotion and hiring restrictions.

The new Governing Board of RBI was appointed in September. With the appointment of the new Board and a new acting director, difficulties were gradually overcome and the much needed review and reorganisation of the Institute structure is now under way.

Despite many discussions on the future directions, during 2004 RBI already achieved a number of important objectives.

In the field of education, the RBI signed agreements establishing cooperation with the University of Dubrovnik (9/2/2004) and the University of Rijeka (5/3/2004). Implementation of these agreements will lead to joint courses of study. Two such courses, involving graduate study in oncology in Dubrovnik and undergraduate study of environmental science in Rijeka, are currently under development.

The difficulty in supporting entering graduate students experienced during 2003 was reversed in 2004 thanks to the generous support of the Ministry of Science, Education and Sport. The RBI was able to recruit forty seven new graduate students thus ensuring that this most important aspect of our educational work continues unabated. Education of graduate students contributes valuable advanced skills to the country and greatly enhances the scientific and applied research conducted at the Institute.

The Institute re-established the tradition of annual Open Days. The 2004 event, held between the 13th and 15th of May, attracted over 3500 visitors. Among them were many distinguished guests such as Stjepan Mesic, the President of Croatia, Dr. Dragan Primorac, the Minister of Science, Education and Sport, and numerous foreign diplomats. The slightly less distinguished, but no less important, guests were comprised of an encouragingly large number of interested school students from all over the country, as well as media personnel, representatives of scientific societies, and delegates from the industrial sector. Apart from the extremely positive response from the public surrounding the entire event, a notable highlight was the concert held in the grounds of the Institute. This concert, organized by members of the Institute in cooperation with the International Women's Club, provided an ideal context in which members of the public (distinguished or otherwise) were able to socialize with employees of the Institute. From opportunities such as this concert, and indeed the entire Open Days event, the general populous was able to get a much better idea of what goes on at the RBI and how it may be applicable to them. In addition to its general utility, it is hoped that events such as these will result in enticing some of Croatia's young and talented minds into the pursuit of the natural sciences, both to further themselves and to brighten the future of country as a whole.

The Institute continues to develop as a national centre where expensive scientific instrumentation is made available to all users within the country and the region. One such example is the NMR centre, which, along

with scientific research, performs service for academic and industrial institutions. The Institute support divisions, the Library and the Centre for Informatics and Computing continue to make important national contributions in development of the scientific information infrastructure and the national CROGRID and EU computational grid.

The RBI remains the only significant source of experimental nuclear-related skills in the country and thus represents a significant strategic resource in view of future energy requirements. Dr. S. Musić, head of the Division of Materials Chemistry was appointed by the president of the Croatian parliament into the Council for nuclear safety. He was also working as a member of Croatian-Slovenian board for monitoring the decommissioning program of the Nuclear Power Plant Krško and the safe disposal of radioactive wastes generated by this plant. This program was successfully completed and accepted by the parliaments of both Croatia and Slovenia.

The RBI Centre for Marine Research in Rovinj continues to coordinate the national marine monitoring and research project Jadran. The project, which engages all national institutions dealing with marine research, is a part of several regional initiatives and discharges Croatian international obligations derived from several ratified documents addressing environmental protection.

As in previous years, the RBI hosted several important international conferences. Among the most noteworthy of these was the FEBS Lecture Course on Cellular Signalling & the 4th Dubrovnik Signalling Conference, held from May 21-27, 2004 and organised by Professor K. Pavelić, In addition, the 9th International Conference on Nuclear Microprobe Technology and Applications, September 13-17, Cavtat, organised by Dr. M. Jakšić and The 19th Dubrovnik International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, June 21-26, Inter-University Centre Dubrovnik, organized by Dr. A. Graovac and Dr. D. Vikić-Topić were major events in the RBI calendar.

The RBI was successful in a number of consortia competing for the EU Framework 6 projects. The awards include projects in development of computing grids, solar energy panels and EU environmental water resources.

Members of the RBI were honoured in international scientific organisations and graduate students received several international prizes. Most notable was the election of Professor K. Pavelić as Vice-President of the prestigious European Molecular Biology Organisation, which has a membership of 1100 distinguished scientists including more than 30 Nobel Prize winners working in this field.

The contributions of RBI staff towards the development of the Institute and the public good were honoured for the first time in the presentation of inaugural Director's prizes. The prizes, which were awarded at the end of the year, recognised the organisation of Open Days, new imaginative advances in teaching and the successful effort in acquiring the funding for the new electron microscope.

Last, but by no means least, the new format of the annual report was introduced in July of 2004. The aim of the booklet was, through the presentation of selected information and examples, to provide a concise overview of the Institute's activity. Particular emphasis was placed upon the top achievements made throughout the year. The interest voiced by the attendees of the First Congress of Croatian Scientists from Croatia and Abroad, for example, was indicative of the success of the new format in promoting the Institute in an appropriate light. It is hoped that this success will become an ongoing characteristic of the report, beginning with the 2004 instalment contained in the subsequent pages.

OVERVIEW

The Ruđer Bošković Institute is the largest Croatian research centre for basic sciences, participating also in science applications and higher education. The multidisciplinary character of the Institute is reflected through the different research fields in physics, chemistry, oceanography (including marine and environmental research and geosciences), biology, biomedicine, computer science and electronics/engineering. With an academic staff of 507, including 284 researchers, 195 Ph. D. students and 28 postdoctoral fellows, the RBI collaborates worldwide with many research institutions and universities.

The Ruđer Bošković Institute consists of twelve divisions, two centres, a library, as well as sections for maintenance, technical services and administration. The main bodies of the Institute are the Board of Governors and the Scientific Council. Their organizational integration with the remainder of the Institute is displayed below (Figure 2).

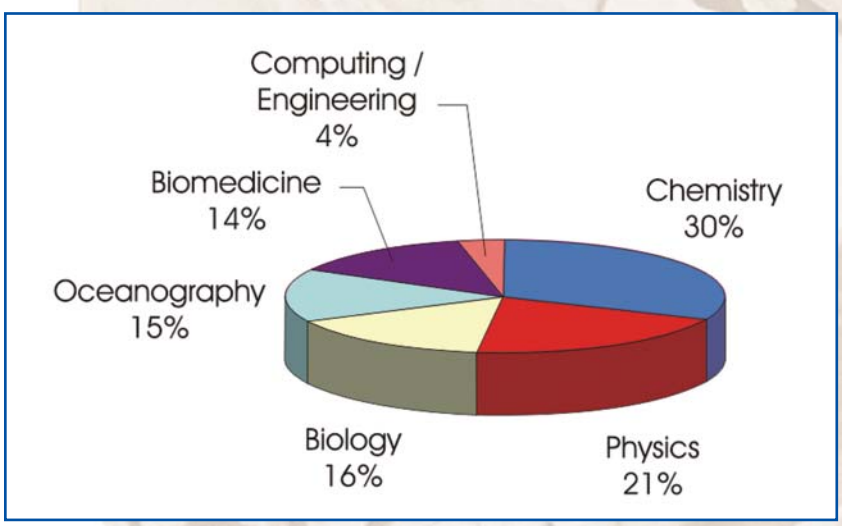


Figure 1. Composition of the academic staff at the RBI

ORGANIZATION OF THE INSTITUTE

Director: Stjepan Marčelja (until November); acting director Mladen Žinić

Head of the Scientific Council: Krunoslav Pisk (untill May); Dražen Vikić-Topić

Chairman of the Board of Governors: Ivo Šlaus (until May); Janko Herak

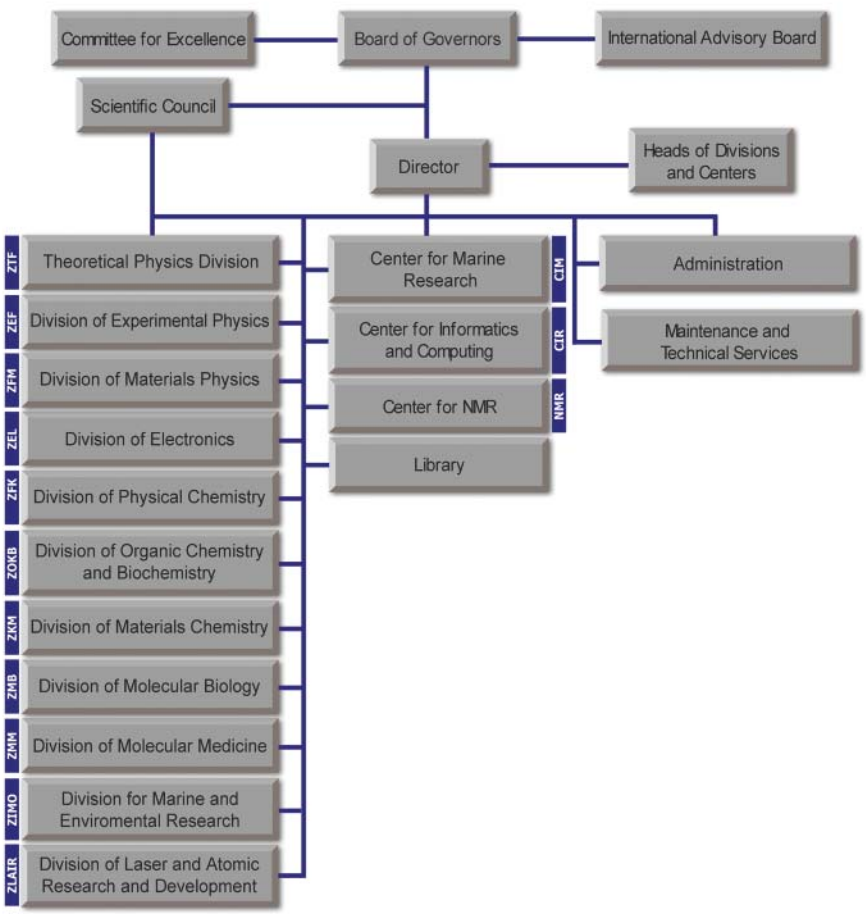


Figure 2. The organisational structure of the RBI

ACTIVITIES

Fundamental research

The total number of research articles published in 2004 was 542. Amongst these, 404 were published in journals cited by Current Contents. With less than 5% of the total number of scientists in the country working at the Institute, it is worthy of note that 27% of all Croatian articles in Current Contents journals originated from the RBI. A considerable proportion of these articles were published in high ranking journals.

Projects

The RBI has 125 projects in basic research which are funded by the Ministry of Science, Education and Sport (MZOŠ). In addition, the Institute is involved with 59 international projects (bilateral, FP6, IAEA, COST etc.), as well as 16 applied and technological projects in cooperation with the World Bank and the MZOŠ.

Higher education

In 2004, scientists from the Institute contributed 63 undergraduate courses and 198 graduate courses to the program of higher education in Croatia. Their respective distributions amongst the five universities at which they were conducted, as well as by the divisions and centres that contributed them are shown in Figures 3, 4, 5, and 6. In addition to the coursework, 25 B.Sc., 14 M.Sc. and 13 Ph.D. theses were completed under the supervision of the RBI academic staff in 2004.

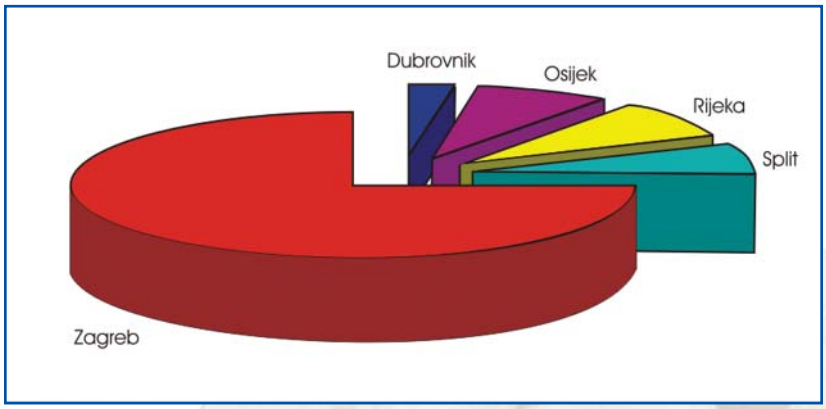


Figure 3. Distribution of the RBI held undergraduate courses (63) by domicile University.

New instrumentation

The RBI received an Atomic force microscope (AFM, Scanning Probe Microscope, VEECO Instruments GmbH, Germany). The AFM provides real topographic images of the sample surfaces in three dimensions with a vertical resolution as small as 1 Å, and with lateral resolution superior to 1 nm, and in «force mode», the movements of the AFM cantilever can be used to measure forces. A wide range of applications includes measuring intra- and intermolecular forces, and measuring the viscoelastic properties of the samples.

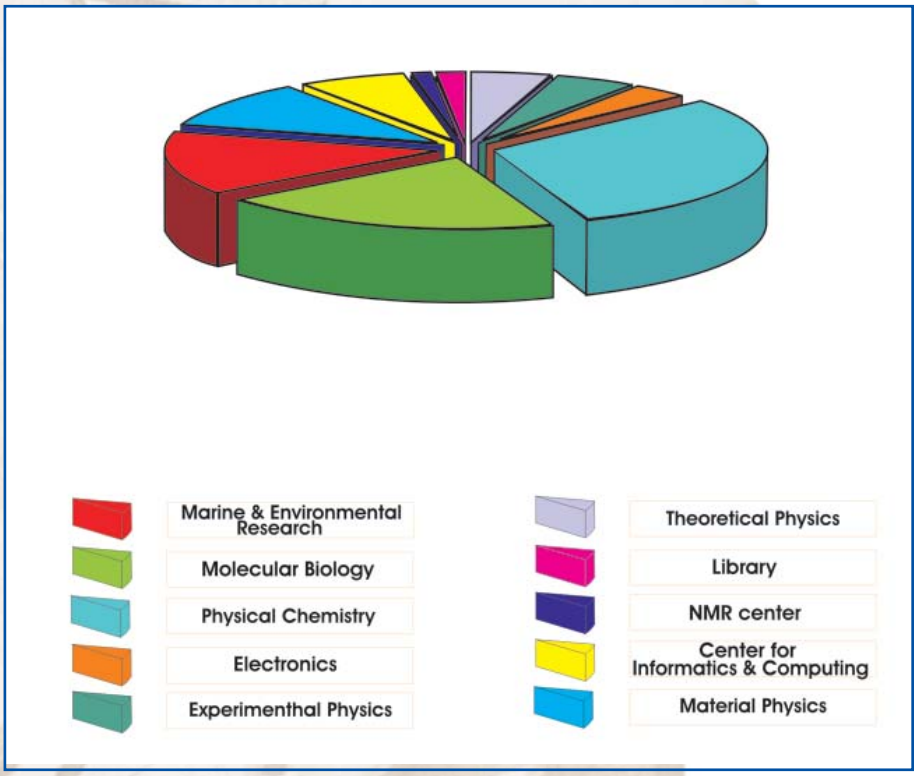


Figure 4. Distribution of the RBI-held undergraduate courses (63) by Divisions and Centres.

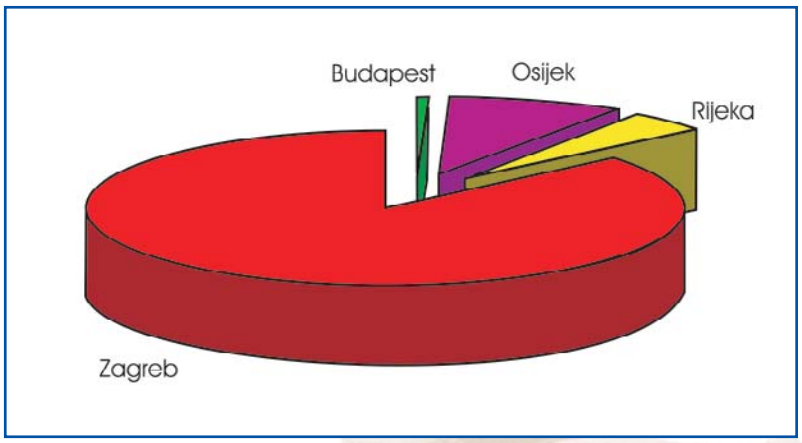


Figure 5. Distribution of the RBI held graduate courses (198) by domicile University

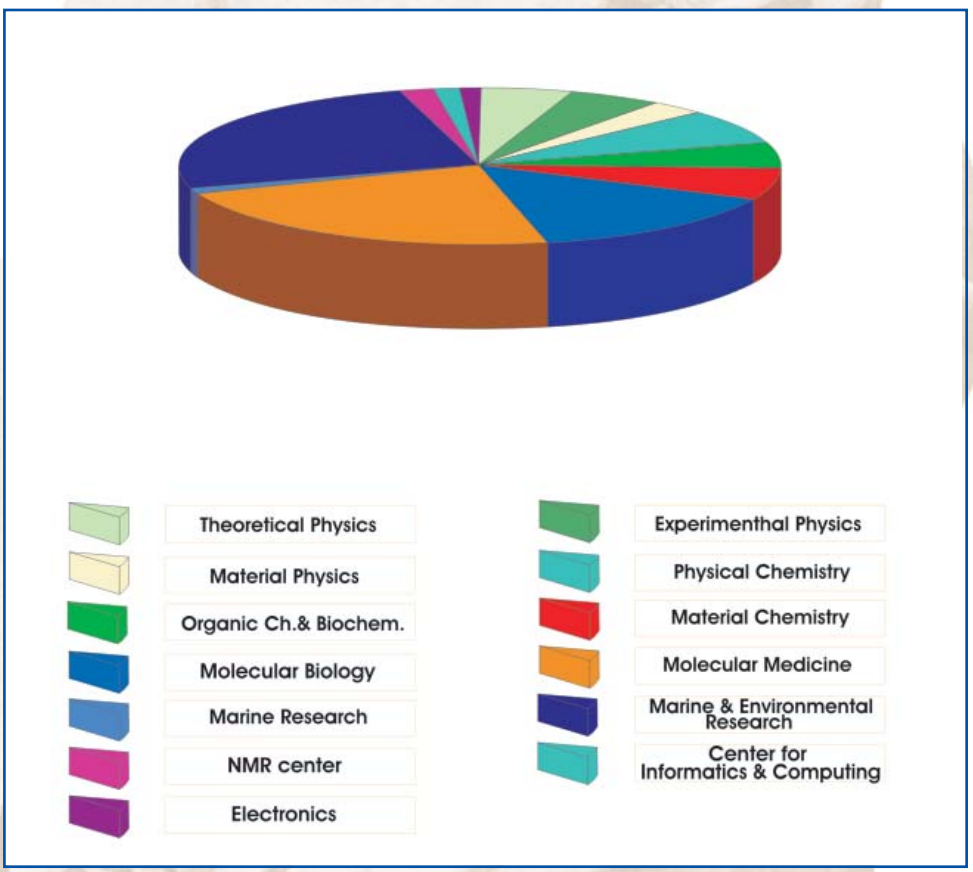


Figure 6. Distribution of the RBI held graduate courses (198) by Divisions and Centres

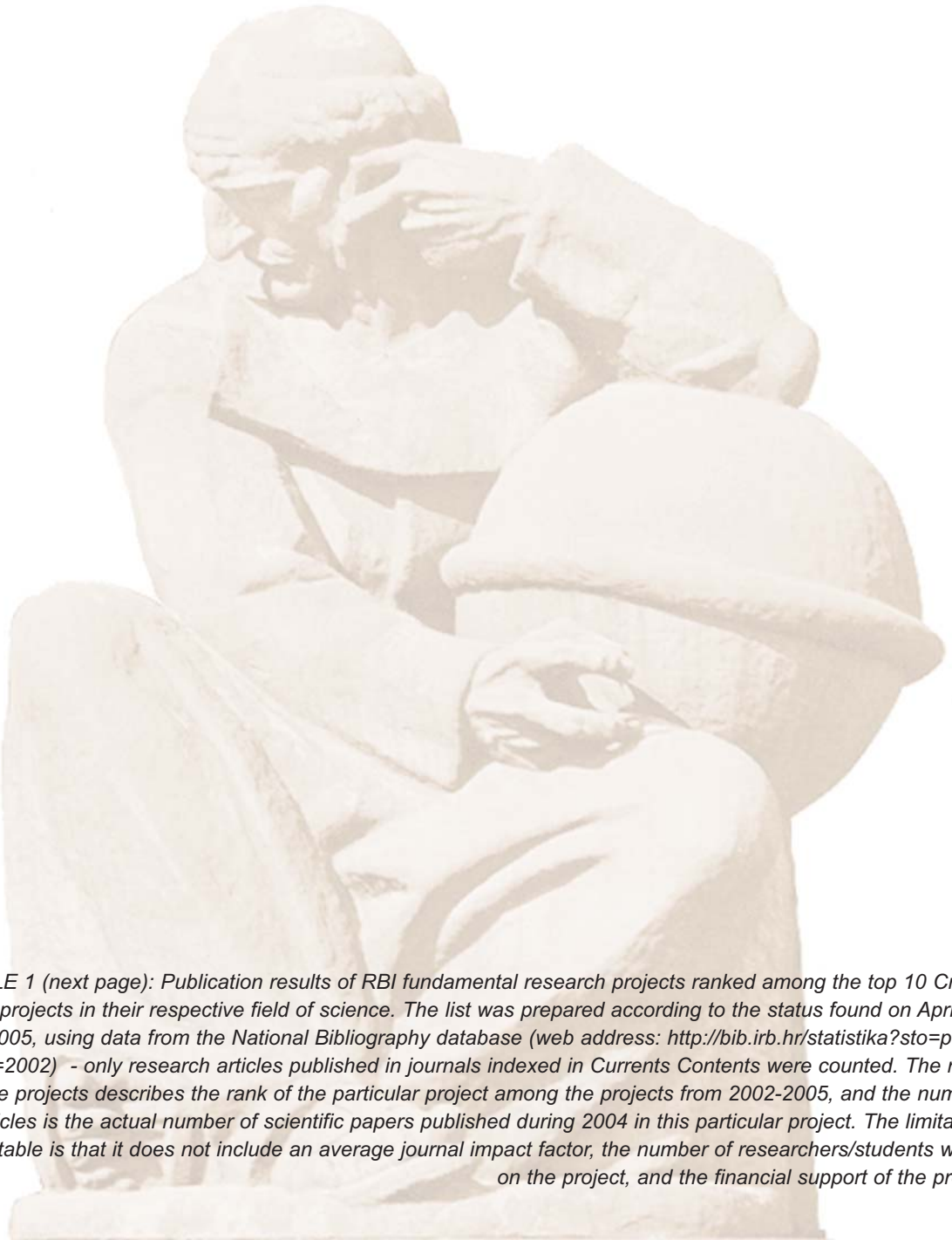
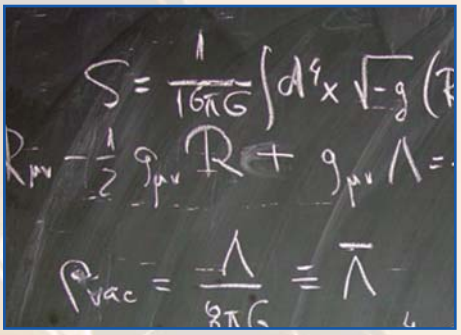


TABLE 1 (next page): Publication results of RBI fundamental research projects ranked among the top 10 Croatian projects in their respective field of science. The list was prepared according to the status found on April 30th, 2005, using data from the National Bibliography database (web address: http://bib.irb.hr/statistika?sto=p&period=2002) - only research articles published in journals indexed in Currents Contents were counted. The rank of the projects describes the rank of the particular project among the projects from 2002-2005, and the number of articles is the actual number of scientific papers published during 2004 in this particular project. The limitation of the table is that it does not include an average journal impact factor, the number of researchers/students working on the project, and the financial support of the projects.

Field of Science – Number of National Projects in the Field	Project Title	Principal Investigator	Rank of the Project in the National Bibliography in 2004	Number of CC Articles Published in 2004
BIOMEDICINE -oncology 72	Influence of gene/protein transduction on signalling pathways of transformed cells	Krešimir Pavelić	1	15
	Gene therapy of tumours by correction of tumour-suppressor genes	Jasminka Pavelić	2	6
	Oxidative stress and malignant diseases	Neven Žarković	3	3
	Regulation of ectopeptidases and opioid receptors expression	Jelka Gabrilovac	8	4
BIOMEDICINE - neuroscience 58	Neuropharmacology of serotonin system	Dorotea Mück-Šeler	1	5
	Molecular pathophysiology of serotonergic transmission	Branimir Jernej	4	6
	Oxidative/antioxidative status after treatment with opioids/opiates	Tanja Marotti	6	3
	Neurotransmitters in stress and regulation of GABA-A receptors in vitro	Danka Peričić	10	1
BIOMEDICINE – chronic diseases 72	Embryonic cell production of pancreatic-like islets	Mirko Hadžija	9	4
BIOLOGY 56	Study of genes and genomes of evolutionary preserved and economically important organisms	Vera Gamulin	4	9
	Dynamics and genetics of bioactive molecules	Volker Magnus	5	6
	Structure and function of plastids and cytoskeleton	Nikola Ljubešić	6	6
	Regulation of recombinant and recombinational repair	Mirjana Petranović	7	4
	Cellular responses to physical, chemical and biological noxis	Maja Osmak	8	4
	The role of recombination in DNA repair and genome stability	Erika Salaj Šmic	10	4
GEOLOGY & OCEANOLOGY 55	Programmed biosynthesis and genotoxic risk	Renato Batel	1	9
	Physics and biogeo-chemistry of trace metals in aquatic systems	Marko Branica	3	8
	Mechanism of long-term changes of the Adriatic-sea ecosystem	Danilo Degobbis	4	7
	Nature and reactivity of organic compounds in seawater and environment	Božena Ćosović	5	5
	Geochemistry of recent and ancient sedimentation systems of the Adriatic platform	Goran Kniewald	6	4
	Persistent organohalogenic pollutants in some costal regions of Dalmatia	Mladen Picer	7	2
	Multidisciplinary sedimentological studies	Halka Bilinski	8	3
	Research on the ebb and long-periodical dynamics of northern Adriatic	Milivoj Kuzmić	9	4
PHYSICS 84	Influence of defects and nanostructures on characteristics of semiconductors	Branko Pivac	2	6
	Fundamental interactions in physics of elementary particles and in cosmology	Branko Guberina	3	19
	Light atomic nuclei: clusters, nuclear molecules, reactions ...	Đuro Miljanić	4	21
	Heavy ion physics	Zoran Basrak	5	17
	Study of nanophase layers and nanocomposite hard electrolytes	Aleksandra Turković	6	4
	Quantum field theory, noncommutative spaces, and symmetries	Stjepan Meljanac	8	6
	High-energy experimental physics	Krešo Kadija	9	12
	Hadronic physics and QCD	Ivan Supek	10	14
CHEMISTRY 74	Proton affinity and proton transfer reaction in chemistry	Zvonimir Maksić	1	16
	Structure and dynamics of (bio)molecules	Biserka Kojić-Prodić	2	15
	Reactivity and reaction mechanisms	Leo Klasinc & Dunja Srzić	3	10
	Reactive intermediates in resting and excited state	Mirjana Maksić	4	9
	Synthesis and microstructure of metal oxides and oxide glasses	Svetozar Musić	5	9
	Development and application of models in chemistry and bioinformatics	Nenad Trinajstić	6	9
	Supramolecular organization in gels, molecular recognition and catalysis	Mladen Žinić	7	8
	Stereoselective synthesis and catalysis	Vitomir Šunjić	8	4
	Electron spin resonance in systems with paramagnetic particles	Boris Rakvin	9	7
	Surfactants, processes in solution and at interfaces	Nada Filipović Vinceković	10	6
ELECTROTECHNICS 74	Analysis of Stochastic Signals, Time Series and Data Structures	Božidar Vojnović	7	0
INFORMATION & COMPUTER TECH. 16	Automated Knowledge Discovery and Reasoning	Nikola Bogunović	1	2

Theoretical Physics Division



http://thphys.irb.hr

DIVISIONAL ORGANISATION

Head: Branko Guberina

Theoretical Physics Division (ZTF) consists of the following laboratories:

- Solid State Physics Group, Radovan Brako
- Particle Physics and Cosmology Group, Neven Bilić
- Theoretical and Mathematical Physics Group, Stjepan Meljanac
- Group for Linear and Nonlinear Dynamics, Mladen Martinis

OVERVIEW OF THE DIVISION

The research performed in the Division is mainly concerned with the theoretical investigation of high-energy physics, such as particle physics, general and mathematical physics, astroparticle physics and cosmology (see Figure 1). In addition, there is a substantial research activity in condensed matter physics. A relatively new and exciting activity in the Division is the application of nonlinear dynamical analysis in biomedicine. In 2004, the members of the Division continued to be involved in lecturing at the University of Zagreb and a number of students completed their B. Sc., M. Sc. and Ph. D. theses.

TOP ACHIEVEMENTS

End of the Universe in a big rip?

The cosmologies with the generalized phantom energy, comprising the phantom energy component with the nonconserved energy-momentum tensor and the space-time dependent Newton constant G, were considered. Large classes of the generalized phantom energy, with very different dynamics of the phantom energy and G, possess the same asymptotic evolution of the Universe depending only on the phantom energy equation of state. In the cosmological model with a growing cosmological term and a variable G, the gravitationally bound systems asymptotically decompose, whereas the nongravitationally bound systems remain bound. This represents the so-called partial rip scenario, as opposed to the big rip effect present in phantom cosmologies (Štefančić H. Phys. Lett. B 2004: 586: 5; Phys. Lett. B 2004: 595: 9).

Pentaquark mass spectrum

Following the revival of the Skyrme model initiated by a recent discovery of pentaquarks, the mass spectra and mass splittings for the higher $SU(3)_f$ representations were calculated in the framework of the minimal $SU(3)_f$ extended Skyrme model. Theoretical estimates were obtained by using only the Skyrme charge as a free parameter and without using any experimental results for the antidecouplet (Duplančić G, et al. J. JHEP 2004: 0407: 027).

Matrix formulation of generalized Calogero-type models

We presented a formulation of generalized Calogero-type models in terms of the matrix oscillator described by the quadratic Hamiltonian and obeying the deformed commutation relations. This formulation provided a description of the multispecies Calogero model, with inverse-square two-body and three-body interactions, without the exchange operators and also made a connection of the Calogero model with quantum Hall physics more transparent (Meljanac S and Samsarov A. Phys. Lett. B 2004: 600: 179; Meljanac S, et al. Phys. Lett. B 2004: 594: 241).

The gluon propagator in the Coulomb gauge

A detailed calculation of the gluon propagator in the Coulomb gauge including finite parts to order g^2 in QCD was performed. The time-time component of this propagator gives interesting results for the colour-Coulomb potential and could provide an unambiguous instantaneous part by using renormalization group arguments (Andraši A. Eur. Phys. J C 2004: 37: 307).

Molecules as electronic devices

Recent advances in experimental methods have made it possible to measure electronic transport through a single molecule bonded onto metal electrodes. Our full ab initio numerical calculations of the oligo phenylene vinylene molecules (OPVn) between gold electrodes reveal nonlinear conductance and its nonexponential decrease with the length of the molecule, complementing the existing experimental data. The theoretical approach uses nonequilibrium electronic structure methods.

Changes in the Hurs exponent of heartbeat intervals during physical activity

The fractal scaling properties of the heartbeat time series were studied in different controlled ergometric regimes. The long-time “memory effect” quantified by the value of the Hurst exponent H>0.5 is found to increase during progressive physical activity in healthy subjects, in contrast to those having stable angina pectoris, where it decreases (Martinis M, et al. Phys. Rev. E 2004: 70: 012903).

SELECTED INVITED LECTURES

1. N. Bilić, "Dark matter and dark energy" invited talk given at the 2004 LHC Days in Split, Split, Croatia, 5-9 October, 2004
2. B. Melić "Charmeless B decays and (non)factorization" invited talk given at the 2004 LHC Days in Split, Split, Croatia, 5-9 October, 2004
3. H. Štefančić, "Phantom appearances of nonphantom cosmologies", invited talk at the 2004 LHC Days in Split, Split, Croatia, 5-9 October 2004
4. I. Andrić, "Matrix model dualities from conformal field theory" invited talk at the Workshop on Quantum Chromodynamics QCD 2004", Paris, France, 7-11 June 2004
5. I. Andrić, "Matrix model duality" invited talk at workshop "What Comes beyond Standard Model", Bled, Slovenia, 19-30 July 2004
6. Z. Škoda, "Noncommutative torsors and quotients", invited talk given at the Workshop Geometric Methods in Algebra and Representation Theory, Warwick, United Kingdom, April 3, 2004
7. Z. Škoda "New and old actions on noncommutative spaces", invited talk given at the Conference NOG II, Quantum Geometry, Mittag-Leffler Institute, Djursholm (near Stockholm), Sweden, May 17, 2004

PROJECTS

Projects supported by the Ministry of Science, Education and Sport:

1. Physics of surfaces, microstructures and strongly correlated systems, Radovan Brako
2. Fundamental interactions in elementary particle physics and cosmology, Branko Guberina
3. Quantum field theory, noncommutative spaces, and symmetries, Stjepan Meljanac
4. Structure of dynamical fluctuations in nonlinear systems, Mladen Martinis

Collaborative projects

1. Radovan Brako: Participation in collaborative project "Nanosciences: A way towards new technologies", MZT, December 2003. Project leader: Dr. M. Milun, Institute of Physics, Zagreb.
2. Kornelija Passek-Kumerički, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Institut für Theoretische Physik II, Ruhr-Universität Bochum, Germany, DFG project "Higher-order QCD corrections in exclusive processes-mesons and baryons".
3. Kornelija Passek-Kumerički, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Institut für Theoretische Physik, Karl-Franzens Universität Graz, Austria, "Hard exclusive photo- and electroproduction of heavy quarkonia".

SELECTED PUBLICATIONS

1. Babić A, Guberina B, Melić B, Štefančić H. Cabibbo-suppressed decays of the Ω_{C0} feedback to the Xic^{+} lifetime. Phys. Rev. D 2004: 70: 117501.
2. Duplančić G, Pašagić H, Trampetić J. Moments of inertia, nucleon axial-vector coupling, the 8, 10, \bar{10} and $27_{3/2}$ mass spectra and the higher $SU(3)_f$ representation mass splittings in the Skyrme model. JHEP 2004: 0407: 027.
3. Štefančić H. Partial rip scenario - a cosmology with a growing cosmological term. Phys. Lett. B 2004: 595: 9.
4. Bakulev AP, Passek-Kumerički K, Schroers W, Stefanis NG. Pion form factor in QCD: From nonlocal condensates to NLO analytic perturbation theory. Phys. Rev. D 2004: 70: 033014.
5. Štefančić H. Generalized phantom energy. Phys. Lett. B 2004: 586: 5.
6. Andraši A. The gluon propagator in the Coulomb gauge. Eur. Phys. J. C 2004: 37: 307.
7. Meljanac S, Samsarov A. Matrix oscillator

and Calogero models. Phys. Lett. B 2004: 600: 179.
8. Meljanac S, Mileković M, Samsarov A. Generalized Calogero model in arbitrary dimensions. Phys. Lett. B 2004: 594: 241.
9. Martinis M, Knežević A, Krstačić G, Vargović E. Changes in the Hurst exponent of heartbeat intervals during physical activity. Phys. Rev. E 2004: 70: 012903.
10. Sekulić B, Martinis M, Nađ K. Estimate of sea loading by pollutants originating from the littoral counties in the Republic of Croatia. Chemistry and Ecology 2004: 20: 437.

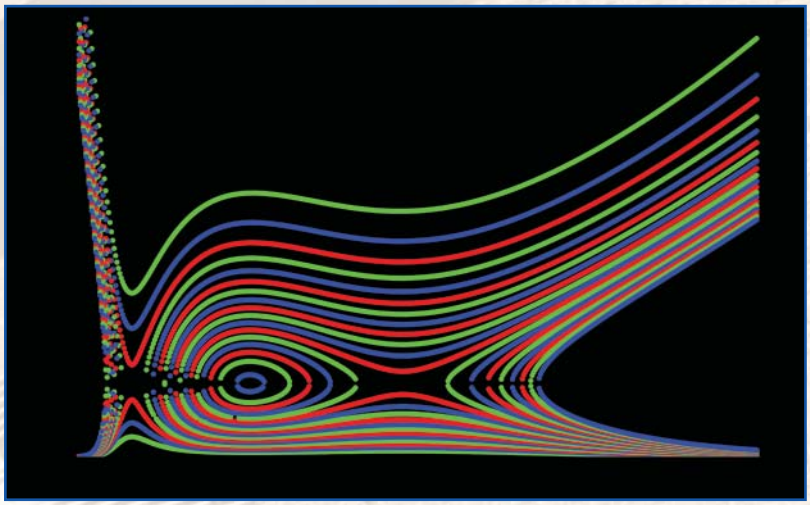
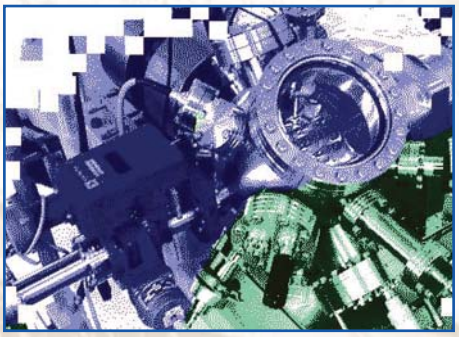


Figure 1: Toplogy of the axisymmetric black-hole accretion.
H. Abraham and N. Bilić.

Division of Experimental Physics



http://www.irb.hr/en/str/zef

DIVISIONAL ORGANISATION
Head: Roman Čaplar until September 2nd
Acting Head: Alfred Švarc from September 3rd

The Division of Experimental Physics (ZEF) consists of the following laboratories:

- Laboratory for nuclear reactions, Đuro Miljanić
- Laboratory for heavy-ion physics, Roman Čaplar
- Laboratory for electromagnetic and weak interactions, Raul Horvat
- Laboratory for ion-beam interactions, Milko Jakšić
- Laboratory for measurement of low-level activities, Bogomil Obelić
- Laboratory for high-energy physics, Krešo Kadija
- Group for the development and the use of analytical methods, Vladivoj Valković

OVERVIEW OF THE DIVISION

In 2004, several ongoing research activities, connected with local as well as international experimental and theoretical research projects, have been pursued. New leading positions in existing international collaborations have been acquired and activities for starting new collaborations were undertaken. Numerous international research contracts have been approved (Framework 5/6, IAEA, NATO), and special effort for obtaining new ones has been encouraged. Important results are achieved in preparing, submitting, implementing and executing technology oriented activities (HITRA).

TOP ACHIEVEMENTS

Experimental high energy physics

An analysis of proton-proton collisions at the CERN NA49 experiment (Figure 1) has been continued with the goal to find exotic baryons with pentaquark structures. Candidates for the Ξ^{--}, Ξ^{0} particles with pentaquark structures were discovered, as well as indication for the existence of their antiparticles.

The second part of the research concerns ALICE, the LHC heavy ion experiment, which will begin taking data in 2008. Fast pulsers necessary for the functioning of the Time Projection Chamber (the ALICE central detector) have been designed and tested with prototypes. There was further development on the already mature IRB ALICE DAQ and Trigger simulation program. An AFFAIR, software for rapid and parallel monitoring of thousands of computers and applications has been developed by our group. A project of setting up the DATA GRID center at SRCE, the University of Zagreb Computing Center, has been also coordinated by our group. The third part of the research involves development and construction of drift chambers for the ATLAS muon spectrometer (LHC experiment, with data taking to start in 2007). (Antičić T, et al., Phys. Rev. C. 2004 : 70 : 034902-1; Alt, C. et al. Phys. Rev. Lett. 2004: 92: 042003-1; Antičić T, et al. Phys. Rev. Lett. 2004: 93: 022302-1)

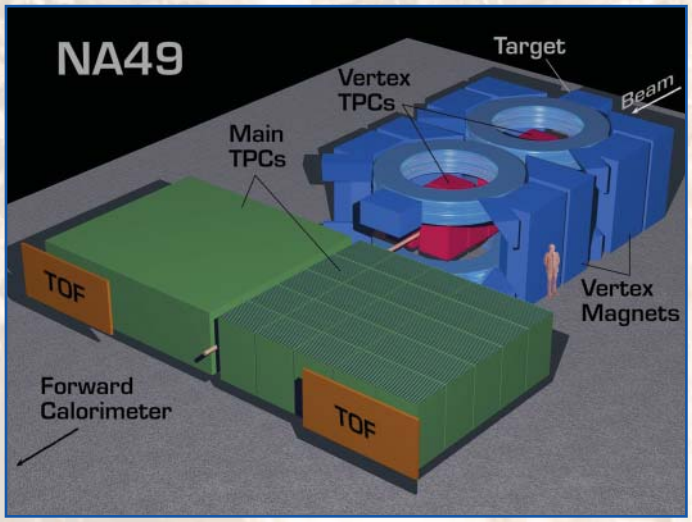


Figure 1: The part of NA49 experimental set-up at CERN (published with the permission of NA49 collaboration).

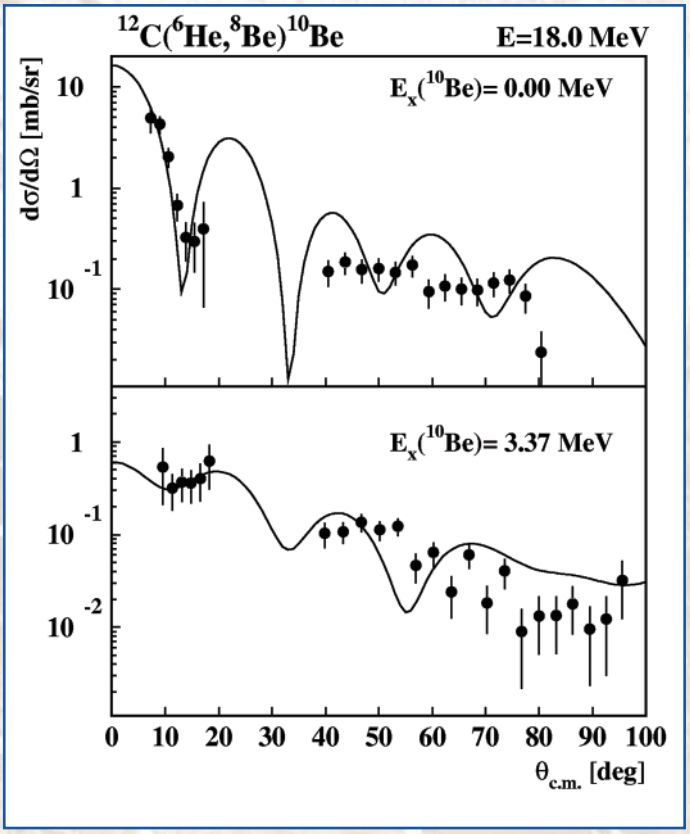


Figure 2:. The experimental angular distributions of the ^{12}C(^{6}He,^{8}Be) reaction forming the ground and first excited state of ^{10}Be compared with the DWBA calculations.

^{6}He reactions with light nuclei

Radioactive ^{6}He nucleus has Borromean structure with two loosely bound neutrons orbiting an α-particle core. Recent availability of the radioactive nuclear beam and the large-area detector arrays (320 strip detectors) at the Institut de Physique Nucléaire, Louvain-la-Neuve, has offered an opportunity for the study of different processes, induced by ^{6}He, of the ^{6}Li, ^{7}Li, ^{12}C and ^{19}F nuclei. In our papers published in 2004, the results are presented for the ^{6}He elastic scattering, as well as the two-neutron stripping, (^{6}He, α), and two-

proton pickup, (^{6}He, ^{8}Be), reactions (Figure 2). The results clearly show the advantages of the reactions for nuclear spectroscopy especially of those states having exotic structure. (Milin M, et al. Phys. Rev. C 2004: 70: 044603-1; Milin M, et al. Nucl. Phys. A. 2004: 730: 285).

Measurement of the rare pion beta decay

The rare pion beta decay $\pi^{+}\rightarrow\pi^{0}e^{+}\upsilon$ is one of the most basic semi-leptonic electroweak processes. It is a pure vector transition between spin-zero members of an isospin triplet, and is therefore analogous to super-allowed Fermi transitions in nuclear β-decay. Due to its simplicity, the theory of Fermi beta decays is one of the most precise components of the Standard Model of electroweak interactions. The PIBETA experiment (Figure 3) measured pion beta decay branching ratio from 1999 to 2001 at Paul Scherer Institute (PSI) and our result for the decay rate $\Gamma_{\pi\beta}$=[0.3980±0.0015(stat)±0.0019(syst)] s^{-1} is in good agreement with Standard Model and Conserved Vector Current (CVC) hypothesis. Using this result, a new value of Cabibbo-Kobayashi-Maskawa (CKM) quark mixing matrix element V_{ud} of 0.9728 has been extracted, which is in excellent agreement with the Particle Data Group (PDG) 2004 average value. (Počanić D, et al., Phys. Rev. Lett. 93: 2004: 181803)

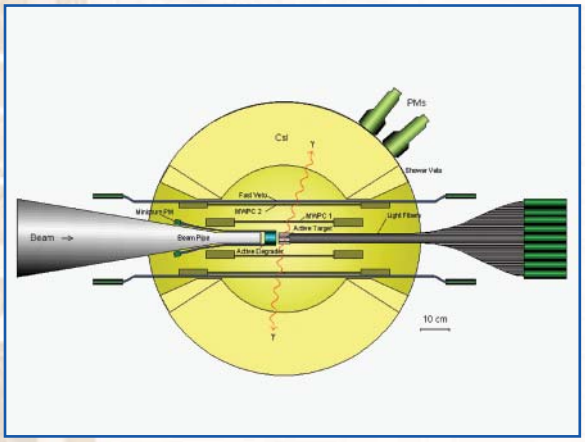


Figure 3:. Shematic presentation of the PIBETA calorimeter at PSI.

PRISMA – New generation detector for nuclear physics

The new magnetic spectrometer PRISMA, the development of which the RBI Laboratory for Heavy-Ion Physics was involved in, has recently entered its operational phase at the Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Legnaro (INFN-LNL), Italy. It has been designed to detect reaction products from heavy-ion collisions, using beams accelerated by the Tandem-ALPI accelerator complex and studying the mass region of A=100-200 mass units. Besides very large solid angle (80 msr) and broad impulse acceptance (~10 %), the PRISMA spectrometer provides, in the range of its mass coverage, resolution of better than one mass unit (1/300) and energy resolution of 0.1 %. This resolution is achieved after the off-line reconstruction of the ion trajectories in a manner similar to that employed in high-energy particle physics. In this way, the fragments of the multi-nucleon transfer reactions, up to the fast fission fragments, are detected with an excellent separation of different isotopes. In order to fully exploit the spectrometer's characteristic high selectivity, an array of γ-radiation detectors (CLARA) is coupled to it. Such performances make

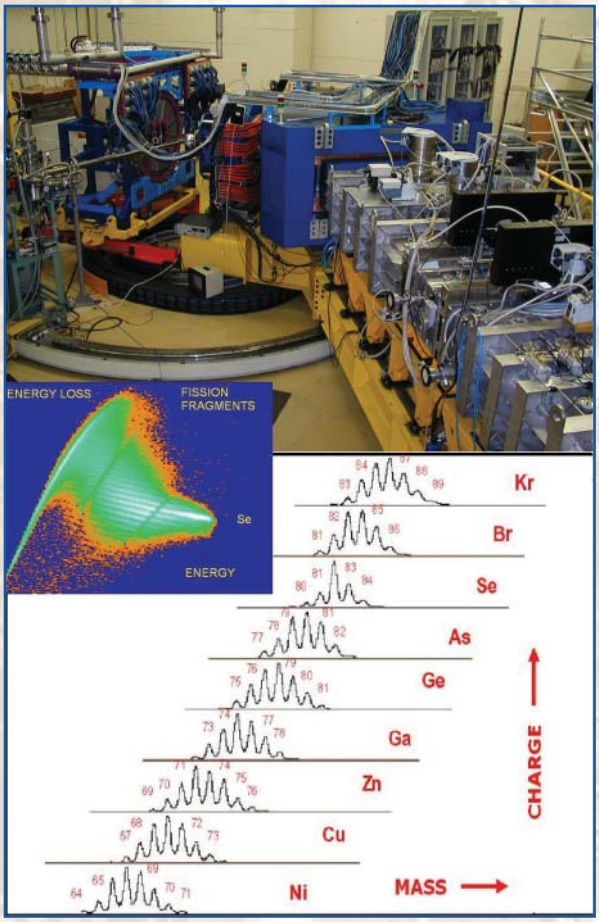


Figure 4:
Upper panel: PRISMA detector (INFN-LNL, Published with permission of the PRISMA collaboration).
Lower panel: Mass distributions of the strongest transfer reaction channels.

PRISMA+CLARA set-up one of the highlights of the new generation nuclear physics detectors.

Search for hadronic axions

An experimental search for the 14.4 keV axions, supposedly emitted from the Sun in M1 transition between the first thermally excited state and the ground state of ^{57}Fe, has been undertaken (Ljubičić A, et al. Phys. Lett. B 2004: 599: 143).

CAST and Large Extra Dimensions

Recent proposals suggest that the weakness of gravity may be evidence for extra dimensions of space. A wide variety of experiments ranging from tabletop probes of Newtonian gravity to searches for microscopic black holes in kilometer-scale detectors are putting these ideas to the test. It has been shown, by a group of scientists from the Ruđer Bošković Institute, that the CERN Axion Solar Telescope (CAST) is capable of probing large extra dimensions with a compactification radius down to 250 nm (Horvat R. et al. Phys. Rev. D 2004: 69: 125011).

Holographic dark energy

Holographic entropy bounds render quantum corrections to the cosmological constant finite, thus providing a natural solution to the cosmological constant problem. It was found that cosmological constant stemming from gravitational holography implies necessarily an interaction of the cosmological constant with the dark-matter sector or a time-dependent Newton's constant to accommodate the observational data (Horvat R. Phys. Rev. D 2004: 70: 087301).

Radiocarbon dating and ecological investigation

The radiocarbon dating by LSC counting method has been introduced and offered by the RBI Laboratory for Measurements of Low-level Radioactivity. Two procedures for sample preparation were developed: benzene synthesis and direct absorption of CO_2. Ecological investigations in Dinaric Karst were continued within the 5th Framework Programme of the EU on the project ICA2-

CT-2002-10009. Radiocarbon dating of several archaeological and geological series from different sites in Croatia and Slovenia was performed.

Installation of new 1.0 MV Tandem accelerator

Through a joint investment of IAEA and Republic of Croatia, a new High Voltage Engineering 1.0 MV tandem accelerator has been installed in 2004. The new accelerator hall is attached to buildings with existing 6.0 MV tandem accelerator and beam lines that include a state of the art nuclear microprobe facility. The new accelerator will be equipped with two ion sources, among which the direct extraction duo-plasmatron ion source has been already installed. The 6.0 MV accelerator has been also upgraded in 2004 by installation of the NEC Alphatross ion source. The production of ion beams with energies above 2 MeV remains.

Figure 5: New 1MV electrostatic Tandem Accelerator.

New technique for 3D imaging of hydrogen

A new detection system for Elastic Recoil Detection Analysis (ERDA), has been installed at the nuclear microprobe facility. The ERDA system has been optimized for detection of hydrogen that can be profiled with depth resolution of 10 nm.

Fast neutron inspection of shipping container

A great deal of effort has been recently invested into the development of the concept of the border management system that keeps pace with expanding trade while protecting from the threats of terrorist attack - "The Smart Border". The shipping container control system is an essential building block of the smart border concept. The proposed novel technique for explosive and fissile material detection makes use of the peculiar capability of producing a tagged neutron beam to confine the inspection to a pre-determined volume element. (Blagus S, et al., Nucl. Instrum. and Meth. B 2004: 213: 434)

CONFERENCES ORGANIZED BY SCIENTISTS OF THE DIVISION

The 9th International Conference on Nuclear

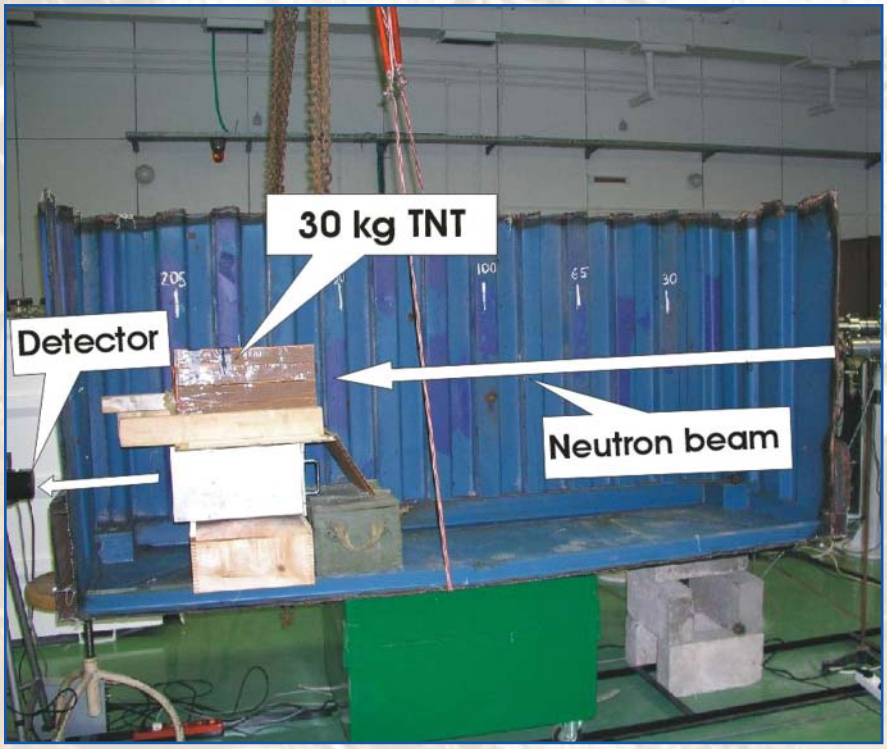


Figure 6: Experimental set-up for the investigations of nature and locations of objects inside the shipping container. Target 30 kg of TNT inside of container.

Microprobe Technology and Applications was held in Cavtat at Adriatic coast from 13th to 17th September 2004, in organization of the Laboratory for ion Beam Interactions (chaired by Milko Jakšić). The Conference was hosted by Croatia after previously organized meetings of this series in United Kingdom, Australia, Sweden, China, USA, South Africa, France and Japan. The conference was attended by scientists from 26 countries, who presented the newest achievements in science and technology using nuclear microprobes.

INVITED LECTURES AT INTERNATIONAL CONFERENCES:

1. T. Antičić, Simulating the ALICE DAQ/ Trigger/HLT, 2004 LHC Days in Split, Split, Croatia
2. V. Brigljević, The CMS High Level Trigger System, 2004 LHC Days in Split, Split, Croatia
3. N. Horvatinčić, Nada, 14C dating of carbonate deposits in the Dinaric Karst, 12th International Karstological School "Clasical Karst", Dating of Cave Sediments, Postojna, Slovenia.
4. M. Jakšić, Nuclear microprobe as a tool for the characterization of radiation detectors, CAARI 2004: 18th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas, USA
5. K. Kadija, Search for exotic baryon resonances in pp collisions at the CERN SPS, International Workshop on PENTAQUARK04, Aioi, Japan
6. M. Stipčević, New directions in quantum cryptography, Internet conference CUC 2004, Zagreb, Croatia
7. T. Šuša, Search for exotic baryon resonances in p+p collisions at the CERN SPS, The XXXIXth Rencontres de Moriond, QCD And High Energy Hadronic Interactions, La Thuile, Italija
8. T. Šuša, Search for pentaquarks, 2004 LHC Days in Split, Split, Croatia

PROJECTS:

Projects supported by the Ministry of Science, Education and Sport:

1. Hadronic physics and QCD, Ivan Supek
2. Light atomic nuclei: clusters, nuclear molecules, reactions ..., Đuro Miljanić
3. Interactions in subatomic and medical physics, Alfred Švarc
4. Heavy-ion physics, Zoran Basrak
5. Massive neutrinos and astro-particles, Ante Ljubičić
6. Photon-atom interactions and correlations, Tihomir Surić
7. Processes of fast ion interactions with matter, Milko Jakšić

8. Natural isotopes of weak activities and development of instrumentation, Bogomil Obelić
9. High-energy experimental physics, Krešo Kadija
10. Methods of explosive, chemical and nuclear material detection, Vladivoj Valković
11. Invariant special relativity and electrodynamics, Tomislav Ivezić

Other projects

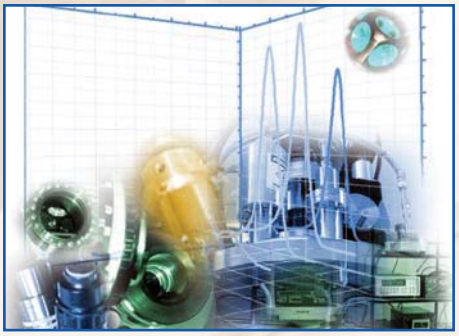
1. Computer aided control of 1.0 MV Tandetron accelerator (Milko Jakšić), MZOS Information Technology Project
2. Applications of nuclear microprobe and synchrotron radiation to characterization of ceramics (Milko Jakšić), bilateral project with China (Institute for High Energy Physics, Beijing)
3. Depth profiling of hydrogen and other light elements in thin films using ERDA spectroscopy (Ivančica Bogdanović Radović), bilateral project with Slovenia
4. Utilisation of ion beam analysis and nuclear spectroscopy techniques in environmental and industrial applications (Milko Jakšić and Bogomil Obelić), IAEA Technical Co-operation project
5. Modular design of the universal ion beam analysis chamber (Milko Jakšić), IAEA Research project
6. Study of anthropogenic pollution after the war and establishing the measures for protection of Plitvice National Park and Bihać region at the border area of Croatia and Bosnia-Herzegovina", European Commission, 5th Framework Programme, (Bogomil Obelić) ICA2-CT-2002-10009
7. Tritium and Stable Isotope Distribution in the Atmosphere at the Coastal Region of Croatia within IAEA CRP F31002 "Isotopic composition of precipitation in the Mediterranean Basin in relation to air circulation patterns and climate (Nada Horvatinčić)
8. Determination of isotopic composition of oxygen and hydrogen in precipitation in ecological and hydrological investigations (Ines Krajcar Bronić), Croatian-Slovenian joint research project
9. Isotopic composition of atmospheric CO2 as an indicator of atmospheric contamination (Ines Krajcar Bronić), Croatian-Slovenian joint research project
10. Investigation of influence of forest ecosystems of National Park Plitvice to the quality of water and lakes (Nada Horvatinčić), National Park Plitvice
11. Inspection of shipping containers for undisclosed radioactive materials (Vladivoj Valković), IAEA, Vienna, Austria.
12. Control of illicit trafficking in threat materials and humans (Vladivoj Valković), NATO project
13. EURITRAC, European illicit trafficking countermeasures kit (Vladivoj Valković), EU FP6 Specific Targeted Research or Innovation Project
14. Feasibility test (Vladivoj Valković), SODERN
15. International collaboration between RBI and MAMI, University of Mainz, Germany on development of frozen spin polarization target (Ivan Supek).

Selected publications

1. Antičić T, et al. Transverse momentum fluctuations in nuclear collisions at 158A GeV. Phys. Rev. C 2004: 70: 034902-1.
2. Alt, C, et al. Evidence for an exotic S =-2, Q =-2 baryon resonance in proton-proton collisions at the CERN SPS. Phys. Rev. Lett. 2004: 92: 042003-1.
3. Antičić T, et al. Lambda and (Lambda)overbar production in central Pb-Pb collisions at 40, 80, and 158A GeV. Phys. Rev. Lett. 2004: 93: 022302-1.
4. Milin M, et al. Two-proton pickup reaction (^{6}He, ^{8}Be) on ^{12}C, ^{16}O, and ^{19}F. Phys. Rev. C 2004: 70: 044603-1.
5. Milin M, et al. The 6He scattering and reactions on ^{12}C and cluster states of ^{14}C. Nucl. Phys. A. 2004: 730: 285.
6. Počanić D, et al. Precise measurement of

the $\pi^+ \rightarrow \pi^0 e^+ \upsilon$ branching ratio. Phys. Rev. Lett. 2004: 93: 181803.
7. Horvat R. Holography and variable cosmological constant. Phys. Rev. D 2004: 70: 087301.
8. Horvat R, Krčmar M, Lakić B. CERN axion solar telescope as a probe of large extra dimensions. Phys. Rev. D 2004: 69: 125011.
9. Ljubičić A, Kekez D, Krečak Z, Ljubičić T. Search for hadronic axions using acioelectric effect. Phys. Lett. B 2004: 599: 143.
10. Blagus S, Sudac D, Valković V. Hidden substances identification by detection of fast neutrons' induced gamma rays using associated alpha particle technique. Nucl Instrum Meth Phys B 2004: 213:434.

Division of Materials Physics



http://www.irb.hr/en/str/zfm

DEPARTMENT ORGANISATION
Head: Branko Pivac

The Division of Materials Physics (ZFM) consists of the following laboratories:

- Laboratory for semiconductors, Branko Pivac
- Laboratory for thin films, Nikola Radić
- Laboratory for molecular physics, Krešimir Furić

OVERVIEW OF THE DIVISION

The research in the Division of Materials Physics is focused on fundamental and applied studies of physical parameters and processes that describe and connect the microscopic and macroscopic properties of condensed matter and molecules. The main goal of the ZFM is to obtain a better understanding of the fundamental characteristics of defects in simple, binary, and multinary semiconductors as well as oxides complementary in semiconductor industry. Certain aspects, such as the mutual interactions of defects, their impact on the relation between microscopic and macroscopic properties of materials, as well as nanophase and glassy material characteristics, prove particularly important. The methods of investigation include the study of amorphous thin films produced by non-thermodynamic processes (magnetron sputtering, ion implantation), particularly Al-W and WC, a-Si and a-Si1-xCx:H films. In addition, the study of processes in magnetron sputtering sources and plasma obtained during laser ablation of metallic and non-metallic materials is undertaken. The ZFM is also involved in fundamental research in the field of molecular and solid state physics with special emphasis on vibrational spectroscopy. The systems under investigation vary in their origin and composition from metals, semiconductors, and ceramics on one side, to molecular crystals and biological samples on the other.

TOP ACHIEVEMENTS

Nanosciences

Nanoscience and/or nanotechnology represent the most promising direction for both modern fundamental scientific research and developments in technology. The Croatian Nanonetwork entitled “Nanosciences: a road to new technologies”, coordinated by M.

Milun (Institute of Physics) was established with the aim of stimulating collaboration amongst different groups having expertise and equipment suitable for research in this field. It involves 7 institutions and 15 formal and 26 international projects. From 22 domestic projects, 4 are lead by B. Pivac, N. Radić, D. Gracin and A. Turković. The collaboration was succesfully continued through 2004.

Selected results in production and study of semiconductor nanocrystals

Germanium quantum dots are of special interest due to their tuneable absorption, intense photo- and electro-luminescence and strong third-order optical nonlinearities; - properties which are very strongly dependent on the size of quantum dots (QD). This makes them very interesting from the fundamental view-point and also potentially suitable for electronic, optoelectronic and photonic applications. Grazing incidence small angle X-ray scattering (Figure 1) at Sinchrotron Elettra, was applied to study the synthesis and growth of Ge QDs in SiO_2 implanted with Ge atoms to high doses, and subsequently annealed.

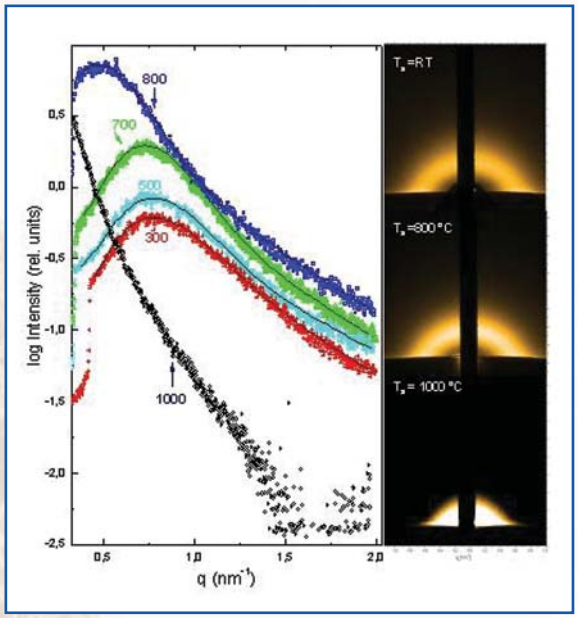


Figure 1. GISAXS results: vertical cross-section of 2D GISAXS spectrum (left) for Ge ion dose D2=6´10^{16} /cm^2, and annealed at various temperatures.

Within collaboration with Technion University, Israel, carbon nanocrystals were produced by implantation of C ions. It appears that under specific implantation/ annealing conditions diamond QDs can be obtained.

Quantum dots have been successfully created on our new magnetron sputtering system. Ge QDs were produced either by co-sputtering of Ge and SiO_2 on hot Si or SiO_2 surfaces or by co-sputtering of Ge and SiO_2 on cold surfaces with subsequent annealing, or by sputtering of Ge on a hot Si surface. Figure 2 shows that, upon choosing suitable conditions of preparation, a well defined Ge QDs can be formed on the surface.

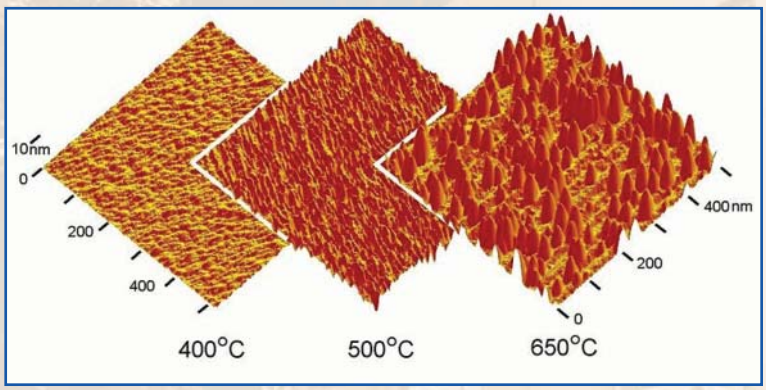


Figure 2. AFM study of Ge QDs formed on Si (100) surface as a function of deposition temperature.

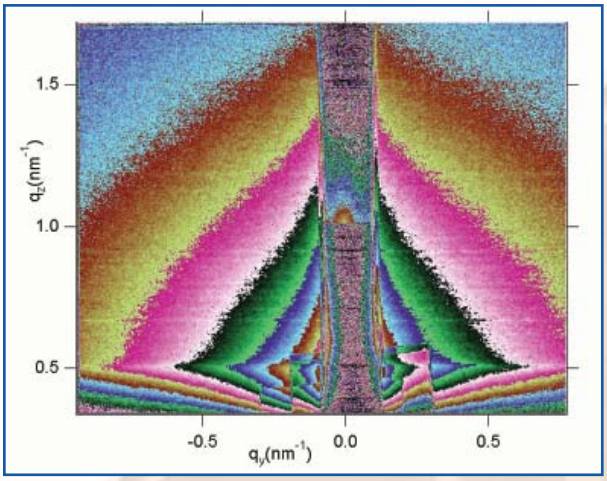


Figure 3. GISAXS 2D-pattern for 55 at % V in V/Ce oxide.

Synchrotron light scattering on nanostructured V/Ce oxide films

Morphology of nanostructured and porous V_2O_5 vanadium oxide, V/Ce oxide and V_2O_5: Li, V/Ce:Li films on glass substrate have been studied by GISAXS (see Figure 3) and grazing-incidence X-ray reflectivity (GIXR) techniques at the ELETTRA synchrotron (Italy, Trieste). With this study, the process of the Li^+ ions' intercalation into the porous, nanostructured films was followed. The particular morphology obtained for certain samples of V in V/Ce oxide is quite suitable for application in electrochromic devices, in an advanced electrochemical cell concept and efficient new solar cells. (P. Dubček et al. J Chem Inf Com Sci 2004:2:1).

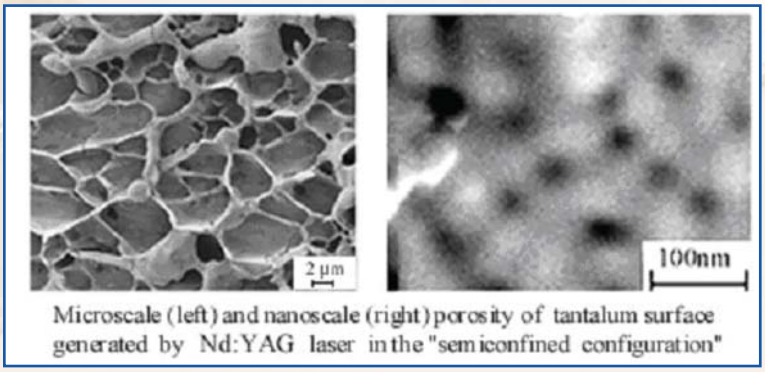


Figure 4. Microscale (left) and nanoscale (right) porosity of tantalum surface generated by Nd:YAG laser in the ``semiconfined configuration``.

Sponge-like Metal Surface Generated by Laser in the Semi-confined Configuration

The applied studies of laser surface modification of materials related to the superheated fluid have resulted in the formation of a deep micro- and nano- porosity of refractory metals. Superheating of tantalum, molilybdenum, up to the spinodal - the point of absolute thermodynamic instability ~ 10^4 K above the boiling point, caused the cascade of bubble explosions and formation of a ~ 10 μm thick porous surface.

PROJECTS

Projects supported by the Ministry of sciences, education and sport:

1. Impact of Defects and Nanostructures on Semiconductor Properties, B. Pivac
2. Magnetron Deposition of Thin Films, N. Radić
3. Physics and Application of Nanostructures, K. Furić
4. Multiphase Amorphous Silicon Alloys as Thin Films, D. Gracin
5. Sugar Hydratation Dynamics, V. Mohaček-Grošev
6. Nanophase Films and Nanocomposite Solid Electrolytes Research, A. Turković
7. Structure and Electrical Relaxation in Glasses and Glass-Ceramics, A. Moguš-Milanković
8. Static and Dynamics of Molecular Solids, D. Kirin
9. Optical Interactions and Organizational Processes in Matter, S. Lugomer
10. Semiconductor Materials for Optoelectronics, B. Šantić

Research and development projects

1. Stress in thin films (N. Radić), (Bilateral collaboration with Slovenia)
2. Study of nanocomposite polymer electrolites (A. Turković), (Bilateral collaboration with Slovenia)
3. Study of disordered materials, nano-optical layers (M. Ivanda), (Bilateral collaboration with Slovenia)
4. Chemically durable iron phosphate glasses for vitrifying stimulated nuclear waste (A. Moguš-Milanković), (IAEA)
5. Hybrid photovoltaic module (D.Gracin) (Ministry of Science, Education and Sport-HITRA-STIRP Project TP-02/0098-35)
6. LPMAS (D.Gracin) (EU- FW6 -INCO- Project No FP6-509178)
7. RISE (Desnica) (EU-FW6-INCO-Project No FP6-509161)

Invited lectures

1. Dr. sc. A. Moguš-Milanković presented plenary lecture entitled “Structure and properties of phosphate glasses” at 13th Slovenian-Croatian Crystallographic Meeting, Bovec, Slovenia, June 16-20, 2004.

NOMINATIONS

1. At the 15th General Meeting of the International Union for Vacuum Science, Technique and Applications (IUVSTA), held in Venice on June 30, 2004, Dr. Branko Pivac was elected to the IUVSTA Executive Council for the 2004-2007 triennium, and Dr. Nikola Radic was confirmed as elected Secretary of the IUVSTA Thin Films Division for the same period.
2. Dr. Branko Pivac was elected member of C8 Committee of The International Union of Pure and Applied Physics.

AWARDS

1. A. Šantić won Commendation Award for research on lead-iron phosphate glasses at The 2004 Younger European Chemists` Conference, Torino, Italy, August 25-29, 2004.

SELECTED PUBLICATIONS

1. Dubček P, Turković A, Crnjak Orel Z, Etlinger B, Bernstdorff S. Synchrotron light scattering on nanostructured V/Ce oxide films with Li+ ions. J Chem Inf Comp Sci 2004: 2: 1.
2. Gracin D, Dubček P, Zorc H, Juraic K. Medium range ordering of amorphous silicon-carbon alloys studied by GISAXS, optical spectroscopy and IBA. Thin Solid Films 2004: 459: 216.
3. Moguš-Milanković A, Šantić A, Karabulut M, Day DE. Electrical conductivity and relaxation in MoO3-Fe2O3-P2O5 and SrO-Fe2O3-P2O5 glasses. J Non-Cryst Solids 2004: 345-346C: 494.
4. Gašparović B, Risović D, Ćosović B. The simple electrochemical method for detection of 3d molecular reorientation in adsorbed layer of organic substances. J Electroanalyt Chem 2004: 573: 391.
5. Ivkov J, Radić N, Tonejc A. Hall effect in Al-W thin films. Solid State Com 2004: 129: 369.
6. Desnica U, Buljan M, Desnica-Franković ID, Dubček P, Bernstorff S, Ivanda M, Zorc H. Direct Ion Beam Synthesis of II-VI Nanocrystals. Nucl Instr Meth Phys Res B 2004: 216: 407.
7. Dubček P, Pivac B, Milat O, Bernstorff S, Zulim I. Study of structural changes in Krypton implanted silicon. Nucl Instr Meth Phys Res B 2004: 215: 122.

Division of Laser and Atomic Research and Development

http://www.irb.hr/str/lair

DIVISIONAL ORGANISATION
Head: Hrvoje Zorc until March 14th
Replacement: Dunja Soldo-Roudnicky

The Division of Laser and Atomic Research and Development (LAIR) consists of the following laboratories:

- Laboratory for Optics and Thin Films, Mladen Pavlović
- Multipurpose workshops, Eduard Švegel

OVERVIEW OF THE DIVISION

The activity of the Division is focused on image and non-image optics as well as on the fundamental aspects of optical thin films. In addition, significant effort is directed toward the application of these basic disciplines in the fields of medicine and defence.

In the medical field, emphasis is placed upon the development of new instrumentation, in particular that relevant to technologies and techniques for photodynamic diagnostics and therapy of skin malignant diseases. Considerable attention is also paid to the implementation of our instrumentation in a clinical setting. This activity, in co-operation with clinics, results in interactive development as well as in optimization of diagnostics and therapy instrumentation and procedures.

The second field of application is directed to the development of instruments for visualization in low visibility conditions. In that sense, we have started a new development project for devices which will be used in night conditions, for needs of national defence as well as in the context of state border monitoring.

TOP ACHIEVEMENTS

Design of optical filters

In the field of thin film optics, reversed design of optical parameters for single, double and multilayered structures was obtained. This was combined with ellipsometry and transmission measurements on many different thin-layer systems. The new designs of optical filters were obtained in co-operation with the Fraunhofer Institute from Jena.

Clinical tests of "MediLED 4"

The major achievement in 2004 was the completion and testing of an advanced computer controlled apparatus for photodynamic diagnosis and therapy (PDT and PDD) of skin malignant diseases under the brand name - "MediLED 4". This device was installed at the "Clinical hospital Split" where it will undergo clinical testing and further optimization of its implementation and diagnosis/therapy protocol will be performed.

Night vision

Besides the optical and medical programs, the division began a new project for development of devices for night monitoring. The new apparatus is based on the last (IV) generation of image intensifier tube. Preliminary testing in night conditions is underway.

Figure 1. Clinical implementation of "MediLED 4" apparatus for PDT/PDD in the "KB Split".

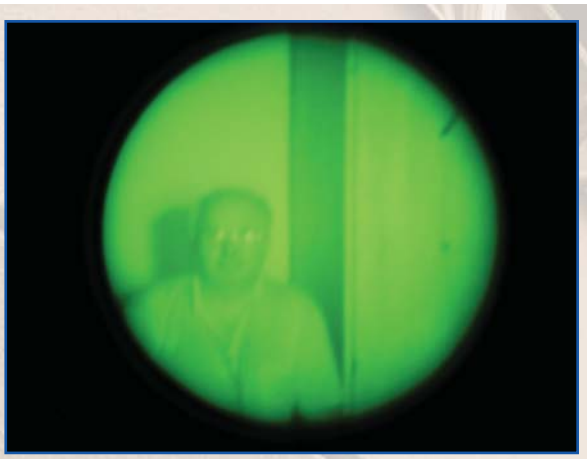


Figure 2. The first results of our new device obtained in the night conditions.

PROJECTS

Project supported by the Ministry of Science, Education and Sports:

1. Photonics of image- and non-image optical systems, Hrvoje Zorc.
2. Light sources for photodynamic therapy of tumours, Anton Peršin. (HITRA-TEST)

Research and development projects

1. Development of night monitoring systems, Dunja Soldo-Roudnicki.
2. Optical instruments and aiming devices - Contract with the Ministry of defense, Hrvoje Zorc.

PATENTS

In 2004 three international patent submissions were applied to The International Bureau of WIPO, 34, chemin des Colombettes, 1211 Geneva 20, Switzerland:

1. Mobile device for photodynamic diagnosis, therapy and methods (PCT/HR2004/000035)
2. Portable illuminator for photodynamic diagnosis (PCT/HR2004/000036)
3. Portable illuminator for photodynamic therapy PCT/HR2004/000037)

AWARDS

In 2004 the division received few awards for developed devices obtained through Ministry of science education and sports project - HITRA. At the ARCA-international exhibition of inventions, held in Zagreb, four of them received awards as the most inventive products. At the Eureka invention exhibition held in Brussels in November 2004, our division was awarded for activities in progress of new Technologies.

Figure 3. Award from the Eureka exhibition.

EDUCATION

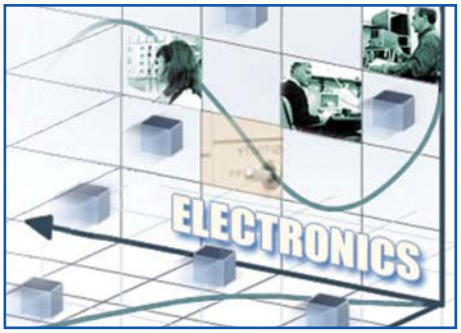
One important activity of the division LAIR is education (four cycles per year) of soldiers for maintenance of optical instruments and aiming devices. This activity is regulated by a contract with the Ministry of defence.

SELECTED PUBLICATIONS

1. Desnica, U., Buljan, M.; Desnica-Franković, I. D.; Dubcek, P.; Bernstorff, S., Ivanda, M., Zorc, H. Direct Ion Beam Synthesis of II-VI Nanocrystals. Nuclear Instruments and Methods in Physics Research Section B. 2004: 216: 407-413
2. Gracin, Davor, Dubček, Pavo; Zorc, Hrvoje; Juraić, Krunoslav. Medium Range Ordering of Amorphous Silicon-Carbon Alloys Studied by GISAXS Spectroscopy and IBA. Thin Solid Films. 2004: 459: 216-219
3. Masetti, Enrico; Bulir, Jiri; Gagliardi, Serena; Janicki, Vesna; Krasilnikova, Anna; Di Santo, G.; Coluzza, C.Ellipsometric and XPS analysis of the interface between silver and SiO_2, TiO_2 and SiNx thin films. Thin Solid Films. 2004: 455-456:468-472
4. Gradišnik,V., Pavlović,M., Pivac,B.,; Zulim,I.: The Transient Photo-dark Current Ratio of a-Si:H p-i-n Photodiode. In: Matijašević, M.; Pejčinović, B.; Tomšić, Ž. Butković Ž, editors. Proceedings of the 12th IEEE Mediterranean Electro technical Conference 2004 May Dubrovnik, Croatia; The Institute of Electrical and Electronic Engineers, 2004. p. 27-29.
5. Janicki,V.,Zorc,H.:Determination of refractive index profile of ZrO_2 on amorphous and pre-evaporated substrates by reverse engineering, In:Amra, Claude ; Kaiser, Norbert,M.,.Angus,H editors. Advances in Optical Thin Films, Proceedings of SPIE, Vol.5250 Washington, USA : SPIE, 2004. p. 546-553.

Figure 4. Testing of the aiming device resolution.

Division of Electronics



http://www.irb.hr/en/str/zel

DIVISIONAL ORGANISATION
Head: Tomislav Šmuc

The Division of Electronics (ZEL) consists of the following laboratories:

- Laboratory for information systems, Dragan Gamberger
- Laboratory for stochastic signals and processes research, Ivan Michieli

OVERVIEW OF THE DIVISION

The Division of electronics has continued to foster research on development of novel intelligent techniques and algorithms for applications in areas of the highest scientific interest. In particular, priority is given to the areas bioinformatics, biomedicine and other real-world applications. With new data acquisition equipment and data and information processing tools, the Division continued to develop common infrastructure for tackling complex scientific and technological problems related to knowledge discovery, pattern recognition and modelling on different sources of data and signals.

Our contribution to undergraduate and graduate education is constantly growing, as is our level of participation in local and international collaborations and workshops.

TOP ACHIEVEMENTS

Data Mining Technology

A novel data classification environment, designed for real-world business problems that exhibit a high degree of undeterministic behaviour, has been devised and implemented. It employs a variation of Naive Bayes algorithm augmented with attribute selection for eliminating redundant attributes. An embedded visual performance evaluation tool enables significantly faster convergence towards the final model.

Data structures and algorithms with application in bioinformatics:

Work on sequence indexing, data retrieval and data compression algorithms has been extended to include free text compression and indexing algorithms for DNA sequences. Adaptive features of previously developed algorithms are used in the development of compact indexing structures.

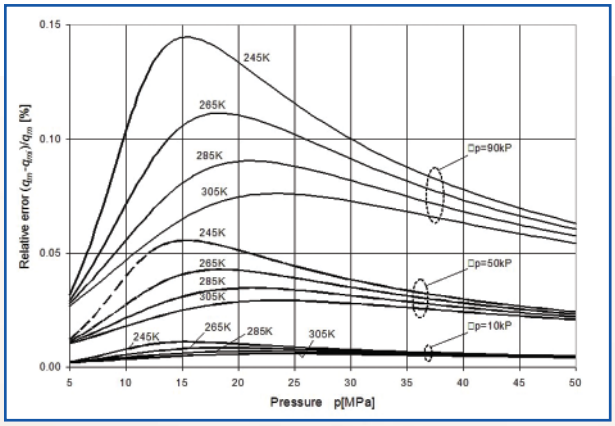


Figure 1. Errors in gas-flow measurement can be corrected using a novel gas isentropic exponent calculation procedure. The procedure can be readily implemented in commercial flow-measurement devices.

Complex measurement systems:

The impact of the isentropic expansion of a natural gas to the accuracy of flow-rate measurements has been investigated. In this context, the corresponding analytical procedure for the calculation of the isentropic exponent, based on a natural-gas-extended virial type characterization equation, is derived. The simulated measurements show considerable effect of the isentropic expansion to the accuracy of flow-rate measurements. It is shown how the corresponding measurement errors can be efficiently compensated by a new procedure (Marić I. et al., Flow Measurement and Instrumentation, 2005: 16: 13).

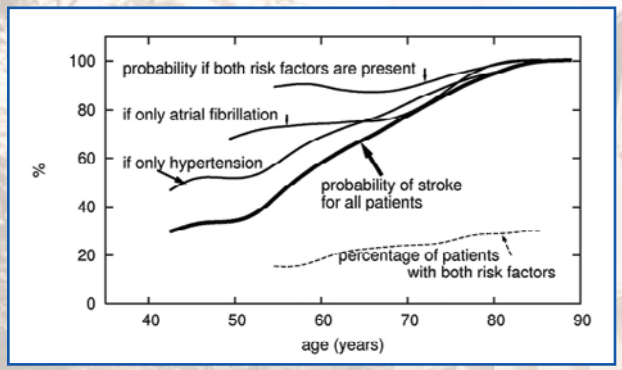


Figure 2. Assessment of the probability of brain-stroke in patients with different risk factors – results obtained using the subgroup discovery methodology.

Educational activities

Knowledge Discovery in Medical Domains, D. Gamberger, Program at the Medical School, University of Zagreb.

Optical communication networks, Lectures (B. Medved Rogina), Faculty of Electrical Engineering and Computing, (FER) Zagreb,

Police operational techniques, Lectures (B. Medved Rogina), Police Academy, Zagreb,

Algorithms in Bioinformatics, Lectures (S. Ristov), postgraduate study, Faculty of Electrical Engineering and Computing, (FER) Zagreb.

New equipment

At the end of the 2004, LISSP acquired new measurement, data acquisition and distributed data processing equipment, consisting of three major components:

- Fast PCI ADC based data acquisition and processing unit;
- Mobile wireless data acquisition system suited for outdoor measurement;
- Cluster processing unit for distributed data processing, based on four dual Xeon 64-bit processors under ROCKS OS supporting EM64T extended 3.3 version.

PROJECTS

Projects supported by the Ministry of Science Education and Sport:

1. Automated Knowledge Discovery and Reasoning, Nikola Bogunović
2. Analysis of Stochastic Signals, Time Series and Data Structures, Božidar Vojnović

Other projects

1. NATO Security Through Science project: Advanced Data- and Knowledge-Driven Methods for State Failure Risk Assessment, (collaboration with University of Ulster, United Kingdom and University of Seville, Spain)
2. Joint Croatian-Slovenian project: Intelligent Data Analysis, Dragan Gamberger, collaboration with J.Stefan Institute, Ljubljana, Slovenia (2004-)
3. Joint Croatian-French project: Intelligent Data Analysis for Decision with Applications in Medicine, Dragan Gamberger, collaboration with University of Lyon, France, IRISA, Rennes, France, and University of Zagreb, Croatia (2004-)
4. Quantum Random Bit Generator, (Branka Medved Rogina, project leader Mario Stipčević, project financed by the World Bank)
5. CRO-GRID, - (Tomislav Šmuc, project leader Karolj Skala, STRIP project, financed by the Ministry of Science Education and Sport)
6. Parallel Random Forests, (Tomislav Šmuc, project leader Goran Topić, financed by the Ministry of Science Education and Sport)

Workshop organization

1. Organization of the Second International Ljubljana-Zagreb Workshop on Knowledge Technologies, November 17-19, 2004,, 2004., Opatija, Croatia.
2. Organization of the Bioinformatika IRB – 2004 workshop, December 10, 2004., Zagreb, Croatia.

Invited talks:

1. Subgroup Discovery Experiments in Functional Genomics, J.Stefan Institute, Ljubljana, Slovenia, 9. 03.2004.by Dragan Gamberger
2. Avoiding Data Overfitting in Scientific Discovery: Experiments in Functional Genomics, University of Lyon, France, 25.11.2004. by Dragan Gamberger.

Products and prototypes

PP-ISO5167 and PP-ISO12213-2: Software packages for flow measurement engineering and natural gas properties calculations (Ivan Marić).

Selected publications

1. 1. Gamberger D, Lavrač N, Zelezny F, Tolar J. Induction of comprehensible models for gene expression datasets by subgroup discovery methodology. J Biomed Inf 2004: 37: 269.
2. Vojnović B, Medved Rogina B. Improvement of Ultra-Wide-Band Signal Timing. In: Biljanović P (ed). Proceedings of the Electronics and Electronic Technologies. Rijeka, Croatia, MIPRO 2004: 124.
3. Vojnović B, Maksimović A. Fractal Signals Characterization Using Fractal Dimension Approach. In: Biljanović P (ed). Proceedings of the Electronics and Electronic Technologies. Rijeka, Croatia. MIPRO 2004: 129.
4. Vojnović, Božidar; Medved Rogina, Branka. Improvement of Ultra-Wide-Band Signal Timing. In Petar Biljanović editor. Proceedings of the Electronics and Electronic Technologies. Rijeka , Croatia, MIPRO 2004. p. 124-128.
5. Vojnović,B.; Maksimović, A. Fractal Signals Characterization Using Fractal Dimension Approach. In Petar Biljanović editor. Proceedings of the Electronics and Electronic Technologies. Rijeka, Croatia. MIPRO 2004. p. 129-132

Division of Physical Chemistry

http://www.irb.hr/en/str/zfk

DIVISIONAL ORGANISATION
Head: Aleksandar Sabljić

The Division of Physical Chemistry (ZFK) consists of the following laboratories:

- Laboratory for Chemical Kinetics and Atmospheric Chemistry, Dunja Srzić
- Laboratory of Radiochemistry, Nada Filipović-Vinceković
- Theoretical Chemistry Group, Tomislav Živković
- Laboratory of Chemical and Biological Crystallography, Marija Luić
- Laboratory for Magnetic Resonances, Boris Rakvin
- Laboratory for Analytical Chemistry, Ivan Habuš

OVERVIEW OF THE DIVISION

Division members have published valuable contributions in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical chemistry, modeling of physical and chemical processes, structural and chemical analyses, and in biosciences. A significant part of this work has appeared in the highest ranking journals in chemistry and biosciences: Journal of Physical Chemistry, Journal of Organic Chemistry, Journal of Geophysical Research, Biophysical Journal, Biological Chemistry, Current Biology. Division members contribute extensively to undergraduate and graduate education and have organized highly regarded scientific conferences. All this is achieved within traditional international collaboration with Harvard University, Rice University, Pacific Northwest Laboratory, Free University Berlin, Hebrew University of Jerusalem, to mention a few.

TOP ACHIVEMENTS

European Tropospheric Ozone Research network

Data obtained during many years of continuous ozone monitoring at 12 selected EUROTRAC-TOR network stations were analyzed by Fourier transformation (T. Cvitaš et al. J Geophys Res-Atmos 2004: 109(D2): 2302). The strong frequency signals are found for the 1 year and 1 day periods. The relative intensity of 1 day peak correlates with the intensity of local photochemical pollution and it was suggested to be used

as its indicator. This analysis also reveals a common variation in ozone volume fractions with quasi-periods ranging between 7 and 44 days. A meteorological data from the station Zugspitze (Germany) showed similar behavior. Thus, these frequencies are most probably due to the quasi-cyclic synoptic scale meteorological influences.

Figure1: Puntijarka air monitoring station near Zagreb at 980 m above sea level.

Efficient method for multiconfigurational systems

An efficient procedure, based on the CASPT2 method using Dunning's correlation-consistent bases and extrapolation to the limit of infinite basis, is proposed for studying difficult multiconfigurational species (I. Ljubić and A. Sabljić. Chem Phys Lett 2004: 385: 214). The procedure is evaluated by calculating the ground state geometry, harmonic wavenumbers and quadratic and cubic force constants of ozone. Its highly multiconfigurational nature makes ozone an ideal candidate for testing the quality of quantum chemical methods. Furthermore, the need for high quality results on ozone steems from its great importance for the atmospheric chemistry and for the life on Earth in general. The geometric parameters obtained are in excellent agreement with experimental data. Calculated wavenumbers as well as quadratic and cubic force constants are very close to the measured values and are comparable to those obtained by computationally far more demanding treatments. The proposed procedure will enable numerous research groups to study the ground and excited states properties of difficult multiconfigurational species since the computational resources at the PC level are sufficient.

Protein-ligand and protein-protein interactions

A novel lipase from Streptomyces rimosus was structurally characterized by MALDI mass spectrometry (I. Leščić et al. Biol Chem 2004: 385: 1147) and its inhibition by various inhibtors was established. The enzyme-ligand interactions for covalently bound inhibitor were determined by mass spectrometry methods (M. Zehl et al. J Mass Spectr 2004: 39: 1474). Modelling of protein-protein interactions involving extracellular ribonuclease barnase and its intracellular inhibitor barstar was performed. Protein engineering and the energy profile of the

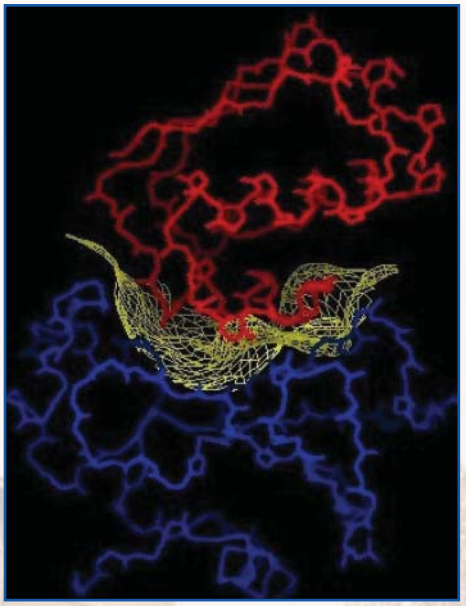


Figure 2: Protein-protein interactions involving ribonuclease barnase (blue) and its inhibitor barstar (red). The binding interface is shown in yellow.

mutant complexes were used to optimize protein binding. (T. Wand et al. Biophys J 2004: 87: 1618)

Designing polymers for sound and vibration damping

Polyurethanes are well-known materials for effective sound and vibration damping. One method for tailoring properties of such materials is the incorporation of selected functional groups. The effect of functional group concentration on phase separation at segmental level was studied by the ESR spectroscopy-spin label method. It was shown that motional heterogeneity, extremely important for the damping efficiency, depends non-linearly on the amount of additional functional groups (J. Čulin et al. Eur Polym J 2004: 40: 1857).

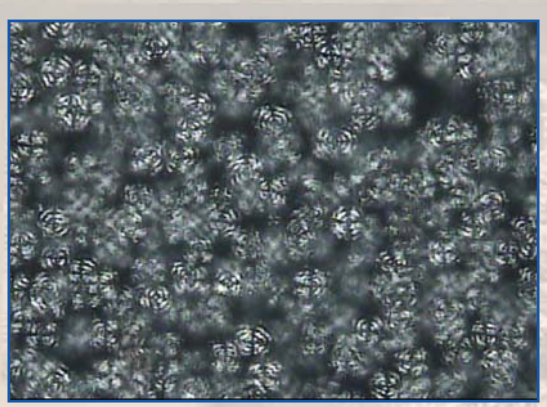


Figure 3: Ring spherulites in polyurethane with functional group concentration of 0.45 millimol per gram as observed by optical microscopy.

PATENT NOVEL BIOCOMPOSITE COATINGS FOR BONE IMPLANTS

Organic-inorganic composite coatings for bioinert implant materials, consisting of calcium phosphate crystals grown “in situ” upon polyelectrolyte multilayers, have been prepared and characterised (H Füredi-Milhofer, P Bar-Yosef, M Sikirić, F Cuisinier, C.Gergely, Organic-inorganic nanocomposite coatings for biological implant materials and methods of preparation thereof, World patent WO 2004/047880 A1, 10.6.2004.). Those coatings consist of several polyelectrolyte multilayers alternating with a few layers of different calcium phosphates (amorphous and/or octacalcium phosphate). The inorganic component seems to be preferable to hydroxyapatite coatings since exchange of the synthetic calcium phosphate with bone mineral is facilitated. Another advantage of newly developed coatings is that bioactive proteins can be co-adsorbed into the organic matrix without losing their bioactivity.

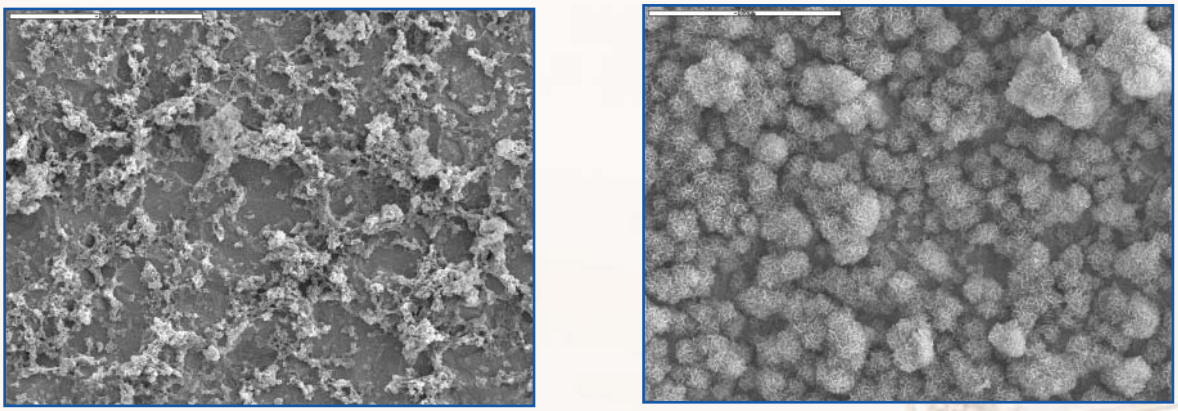


Figure 4: Organic-inorganic composite coatings for bioinert implant materials. Organic component consists of multilayers of poly-L-Lysine and poly-L-glutamicacid. The inorganic components are (a) amorphous calcium phosphate and (b) octacalcium phosphate.

EDUCATIONAL ACTIVITIES

Division provides anually over 30 undergraduate and graduate courses at Universities in Zagreb, Split, Rijeka and Osijek.

AWARDS

1. Nenad Trinajstić, Life Achievement Award for outstanding contributions in Natural Sciences awarded by the Croatian Parlament
2. Nenad Trinajstić, The Božo Težak Medal, Croatian Chemical Society
3. Zoran Štefanić was awarded by The Cambridge Crystallographic Data Centre for the best poster presented at the 22nd European Crystallographic Meeting, Budapest, Hungary, 26-31 August 2004.

SELECTED COLLABORATIONS

1. COST chemistry D-27 action "Origin of Life and Early Evolution", Vesna Noethig-Laslo
2. COST chemistry D-22 action "Protein-Lipid Interactions", Greta Pifat-Mrzljak
3. COST physics P-15 action "Advanced Paramagnetic Resonance Methods in Molecular Biophysics", Boris Rakvin
4. "Ultrafast and ultracold experimental and theoretical methods and applications" Collaborative project supoported by Ministry of Science, Education and Sport
5. UNESCO-CEPES project "Brain drain and the academic and intellectual labour market in south east Europe" Greta Pifat-Mrzljak
6. "Synthesis, structure, and mechanisms of fuctional molecules and supramolecular systems" Collaborative project supoported by Ministry of Science, Education and Sport

SELECTED INVITED LECTURES

1. S.D. Bosanac "Atom-Molecule Energy Transfer in Confinement", Harvard University (ITAMP), Cambridge, MA, U.S.A., 6 February 2004.
2. M. Sikirić "Aditive Interactions with Calcium Hydrogenphosphate Dihydrate", Bat Sheva Workshoop on Biomineralization, Mashabei Sadeh & Eilat, Israel, 22 February 2004.
3. M. Bonifačić "Oxidation Mechanism of Aliphatic Amino Acids as Studied by Time-Resolved Methods", Graduiertenkolleg Symposium 2004, Universität Leipzig, Leipzig, Germany, 2 June 2004.
4. G.Pifat-Mrzljak "National Case Study: Brain Drain and the Academic and Intellectual Labour Market in Croatia", UNESCO conference, Bucharest, Romania, 18-19 June 2004.

CONFERENCES ORGANIZED BY SCIENTISTS OF THE DIVISION

1. 19th MATH/CHEM/COMP, Dubrovnik, 21-26 June 2004
2. 9th Brijuni Conference "Matter under extreme conditions", Brijuni, 3 September 2004

PROJECTS

Basic research projects supoported by the Ministry of Science, Education and Sport:

1. Properties and behaviour of atmosferic microconstituents, Tomislav Cvitaš
2. Surfactants, processes in solution and at interfaces, Nada Filipović-Vinceković
3. Reactivity and reaction mechanism, Dunja Srzić
4. Investigation on chemical reactivity and ultrafast processes, Aleksandar Sabljić
5. Development and application of models in chemistry and bioinformatics, Nenad Trinajstić
6. Structural and biological investigation of new complex compounds, Ljerka Tušek-Božić
7. Structure and dynamics of (bio)molecules, Biserka Kojić-Prodić
8. Biophysics of liporotein interactions with active substances, Greta Pifat-Mrzljak
9. Electron spin resonance in systems with paramagnetic particles, Boris Rakvin
10. Modeling of novel carbon materials, Ante Graovac
11. Interactions of biomembranes with amino acids and peptides, Vesna Nöthig-Laslo
12. Multidisciplinary sedimentological investigations, Halka Bilinski
13. Matter under extreme conditions, Slobodan Bosanac
14. Description and behaviour of quantum systems in interaction, Tomislav Živković
15. Synthesis of peptide libraries-analytical methods and combinatorial chemistry, Ivan Habuš

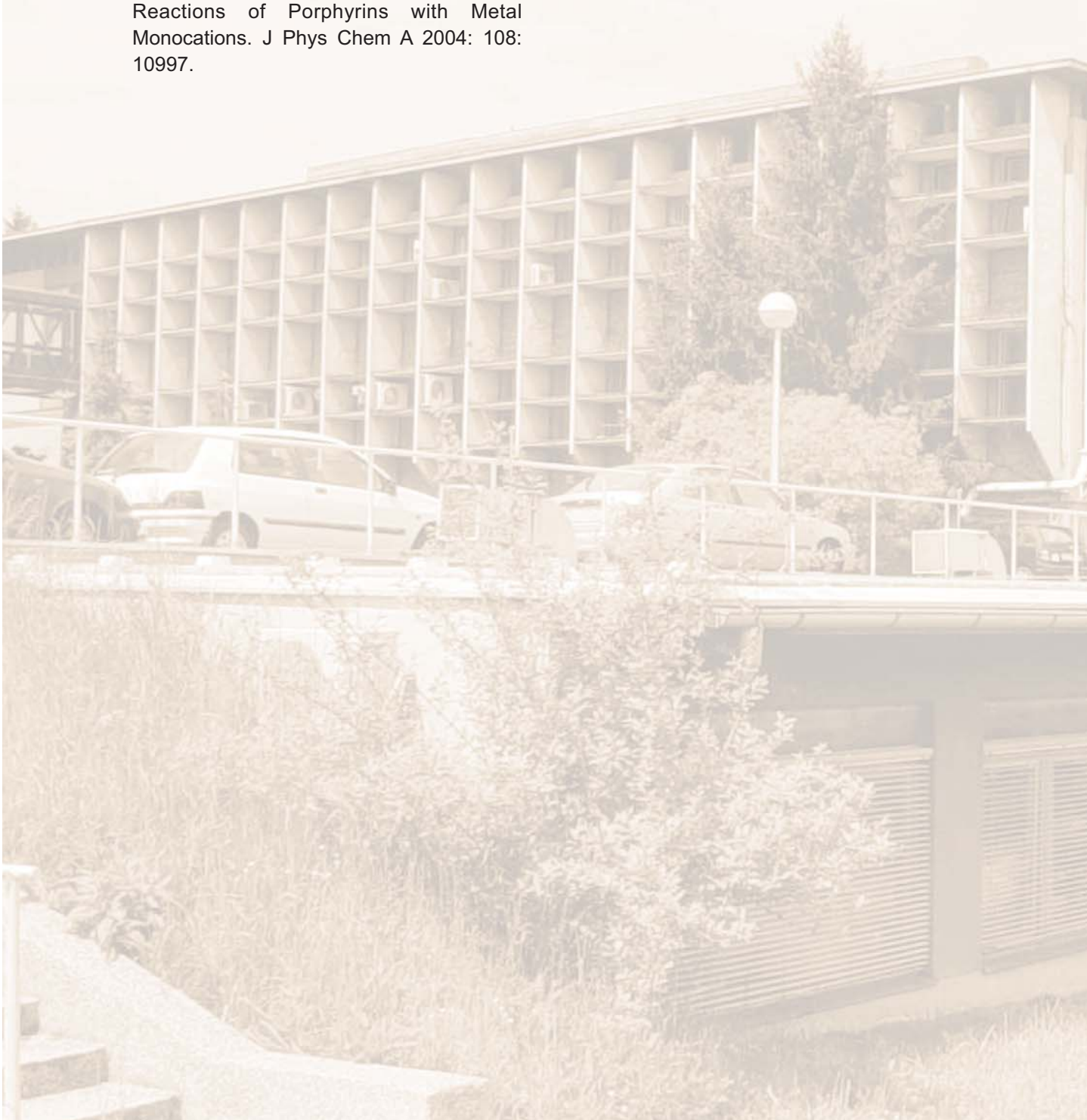
Other projects

1. Prediction of enzyme selectivity, regulation, and inhibition by COMBINE analysis, S. Tomić (Bilateral project with Germany)
2. Structure and dynamics of interpenetrating polymer networks, M. Andreis (Bilateral project with Slovenia)
3. Structure and Dynamics of Biomolecules, M. Luić (Bilateral project with Slovenia)
4. Interaction of biomembrans with peptides, V. Noethig-Laslo (Bilateral project with Slovenia)
5. Cell membranes and oxidative stress, G. Pifat-Mrzljak (Bilateral project with Slovenia)
6. Structural investigation of natural polymers and complexes by mass spectrometry, D. Srzić (Bilateral project with Slovenia)
7. Combined quantum mechanical and force field approaches in study of molecules of biological and biotechnological interest, S. Tomić (Bilateral project with Slovenia)

SELECTED PUBLICATIONS

1. Wang T, Tomić S, Gabdoulline R, Wade R. How optimal are the binding energetics of barnase and barstar? Biophys J 2004: 87: 1618.
2. Leščić I, Zehl M, Müller R, Vukelić B, Abramić M, Pigac J, Allmaier G: Structural characterization of extracellular lipaze from Streptomyces rimosus: Assignement of disulfide bridges pattern by mass spectrometry. Biolog Chem 2004: 385: 1147.
3. Novak I, Harrison LJ, Kovač B, Pratt LM. Electronic Structure of Persistent Radicals: Nitroxides. J Org Chem 2004: 69: 7628.
4. Cvitaš T, Furger M, Girgzdiene R, Haspra L, Kezele N, Klasinc L, Planinšek A, Pompe M, Prevot A, Scheel HE, Schuepbach E. Spectral Analysis of Boundary Layer Ozone Data from the EUROTRAC TOR* Network. J Geophys Res -Atmos 2004: 109(D2): 2302
5, Tarabek P, Bonifačić M, Beckert D. Photooxidation of Glycylglycine. Indication of Two-channel Reaction Mechanism by

Time-resolved FT EPR. J Phys Chem A 2004: 108: 3467.
6. Piližota T, Lučić B, Trinajstić N. Use of variable selection in modeling the secondary structural content of proteins from their composition of amino acid residues. J Chem Inf Comput Sci 2004: 44: 113.
7. Kazazi S, Klasinc L, McGlynn SP, Srzić D, Vicente MGH. Gas-phase Metallation Reactions of Porphyrins with Metal Monocations. J Phys Chem A 2004: 108: 10997.
8. Tolić-Nørrelykke M, Sacconi L, Thon G, Pavone FS. Positioning and elongation of the fission yeast spindle by microtubule-based pushing. Curr Biol 2004: 14: 1181.
9. Ljubić I, Sabljić A. CASPT2 systematic analysis on the geometry and force field of ozone with extrapolation to the infinite basis limit. Chem Phys Lett 2004: 385: 214.



Division of Organic Chemistry and Biochemistry

http://www.irb.hr/en/str/zokb

DIVISIONAL ORGANISATION

Head: Mladen Žinić / Kata Majerski

The Division of Organic Chemistry and Biochemistry (ZOKB) consists of the following laboratories:

- Laboratory for stereoselective catalysis and biocatalysis, Zdenko Hameršak
- Laboratory for synthetic organic chemistry, Kata Majerski
- Laboratory for supramolecular and nucleoside chemistry, Mladen Žinić
- Laboratory for carbohydrate, peptide and glycopeptide chemistry, Štefica Horvat
- Laboratory for cellular biochemistry, Marija Abramić
- Laboratory for physical organic chemistry, Mirjana Eckert-Maksić
- Laboratory for molecular spectroscopy, Goran Baranović
- Group for quantum organic chemistry, Borislav Kovačević

OVERVIEW OF THE DIVISION

In 2004, the Division of Organic Chemistry and Biochemistry made several important discoveries in a broad range of topics such as synthetic and physical organic chemistry, stereoselective synthesis and catalysis, supramolecular chemistry, peptide and glycopeptide chemistry, molecular spectroscopy, protein biochemistry and quantum organic chemistry. A significant number (55) of these contributions were published in high ranking and leading chemical journals. The scientists of the division also made a significant contribution to higher education in organic chemistry by providing 9 courses at undergraduate and postgraduate levels and by supervising a number of Diploma theses, M.Sc. and Ph.D. theses.

TOP ACHIEVEMENTS

Quantum organic chemistry

Studies of the stable doubly-charged positive molecular ions formed by direct attachment of alpha particles to HCN and HNC showed that $[HeNCH]^{2+}$ and $[HeCNH]^{2+}$ are metastable dications with a very long life-time (Figure 1). They should exist in the

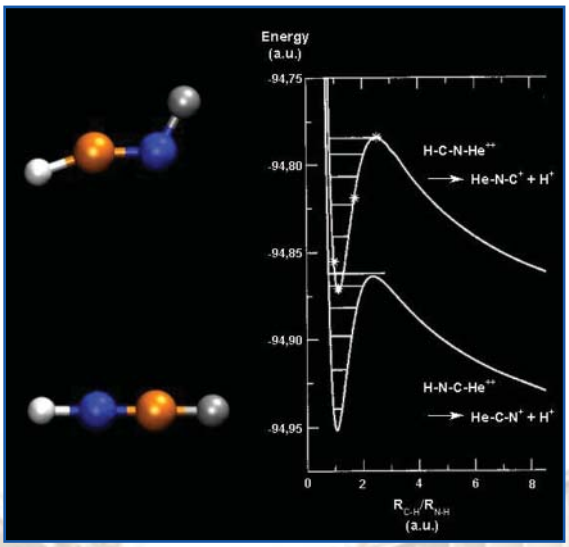


Figure 1. Potential energy curves for the proton loss processes of $[HeNCH]^{2+}$ and $[HeCNH]^{2+}$ dications.

interstellar space and comets. (A. Palacios at al.,Phys Rev Lett 2004: 92: 133001).

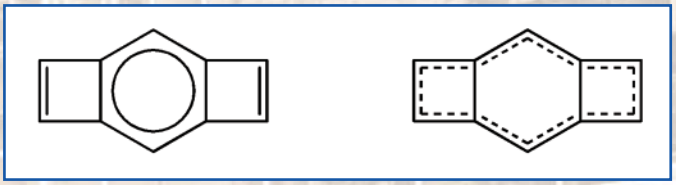
An extensive study of the origin of aromaticity provided the best in-depth analysis carried out so far while offering new insight into the physical nature of the chemical phenomenon called aromaticity. It has been shown convincingly that the extrinsic aromaticity is a consequence of the σ-molecular framework in archetypal benzene, which represents a Copernicus' reversal in interpreting this important cornerstone of organic chemistry. (B. Kovačević at al. Chem Phys Chem 2004: 5: 1352).

Supramolecular chemistry of gels

In collaboration with French and German groups a series of oligoamide gelators has been prepared which displayed remarkable gelation properties in organic solvents and water opening a wide range of possible applications. (A. D'Aleo at al. Chem Communications 2004: 190-191).

Bond-Stretch Isomerism in Organic Molecules

The notion of bond-stretch isomerism was introduced by Chatt in order to characterize metallic complexes, which differ only by length in one or several bonds. However, the experimental evidence proved inconclusive. Advanced multireference coupled-cluster MR-AQCC/6-31G(d) calculations provided, for the first time, strong evidence that benzo-(1,2:4,5)dicyclobutadiene exists in two isomeric forms 1 and 2 degenerate in energy and separated by a barrier of 5 kcal/mol. They differ only in their CC bond distances. The isomer 2 has a form of the highly elusive quasi-(10) annulene. (I. Antol et al. Chem Phys Chem 2004: 5: 975).



a b

New methods in organic synthesis

Hitherto unknown tin-templates were prepared. (I. Vujasinović at al. J Org Chem 2004: 69: 8550). These compounds are very useful building blocks for the synthesis of various macrocyclic polythiaether-polythiaester ligands (Figure 2a).

Also, novel the synthesis of novel organogermanium compounds via metallation of 3-trimethylsilyl-3-ethoxycarbonylcyclopropene derivatives was developed (I. Zrinski at al. Organometallics 2004: 23: 2806, Figure 2b).

In addition, novel chiral diaryl aziridines were synthesized using enantiopure ylides,

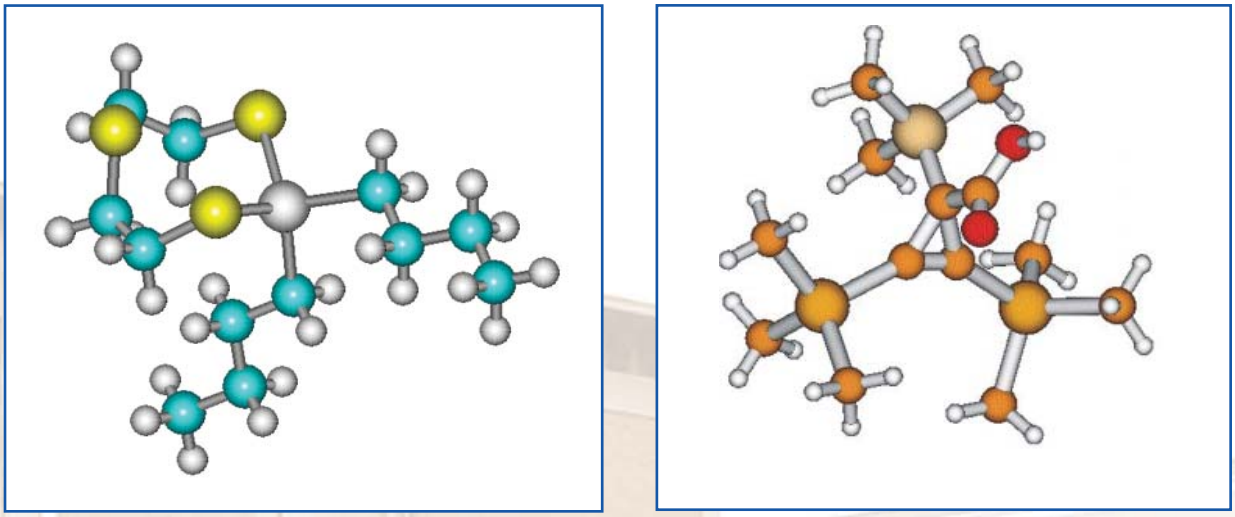


Figure 2. Structures of:
a) Tin-template 2,2-dibutyl-2-stanna-1,3,6-trithiacyclooctane
b) 1,2-Bis(trimethylgermyl)-3-trimethylsilyl-3-carboxycyclopropen

derived from Eliel`s oxathiane and phosphazene base. (A. Solladié-Cavallo et al. J Org Chem 2004: 69: 1409).

Protein biochemistry

The extensive comparative in vitro study of a cytosolic zinc aminopeptidase (dipeptidyl peptidase III, DPP III) from two mammalian species (human and rat), has revealed the striking inter-species difference in the reactivity of protein sulfhydryl (cisteinyl) residues important for the substrate binding (M. Abramić et al. Int J Biochem Cell Biol 2004: 36: 434). The obtained experimental results, supported by the bioinformatic analysis, indicate, for the first time that the in vivo reversible redox regulation could be of physiological significance for this type of eukaryotic metallo-peptidase, and that a regulatory residue might be the only phyllogenetically 100% conserved Cys (Figure 3.).

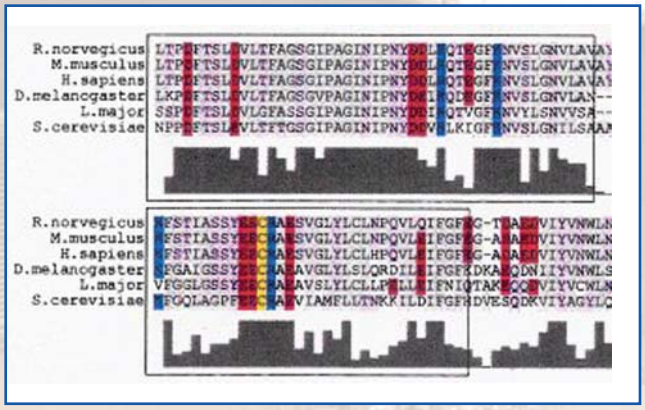


Figure 3. Partial alignment diagram of 6 eukaryotic DPP III sequences showing two out of five conserved amino acid sequence regions and the only 100% conserved Cys (printed black on yellow), corresponding to the position 509 in human DPP III sequence.

AWARDS

1. Borislav Kovačević was awarded The Croatian state annual award for young scientists in the field of natural sciences.
2. Robert Vianello received the Annual award of the City of Rijeka for his scientific work as well as an Annual award of The Society of University Teachers and Scientists, Zagreb, Croatia for young scientists.
3. Ina Nemet and Maja Roščić also won Annual awards for young scientists of The Society of University Teachers and Scientists, Zagreb, Croatia.

PROJECTS

International and collaborative projects

1. Photoinduced Proton Transfer in Biologically Active Molecules - Theoretical Investigation, Bilateral Croatia-Austria project, M. Eckert-Maksić.
2. Properties of new molecular materials, Working group within COST D26, M. Eckert-Maksić.
3. Thermally processed foods: possible health implication, Management Committee and Working group within COST 927, Š. Horvat.
4. Simulation of Proton Dynamics in Systems of Biological Interest, Bilateral Croatia-Slovenia project, Z. Maksić.
5. Intrinsic Reactivity of New Molecular Materials, Working group within COST D26, Z. Maksić.

Projects supported by the Ministry of Science, Education and Sport:

1. Stereoselective synthesis and catalysis, Zdenko Hameršak
2. New optically active materials, Vladimir Vinković
3. Synthesis, molecular structure and function of polycyclic molecules, Kata Majerski
4. Supramolecular organization of gels, molecular recognition and catalysis, Mladen Žinić
5. Design and synthesis of bioactive peptides, glycopeptides and biomarkers, Štefica Horvat
6. Reactive intermediates in ground and excited state, Mirjana Eckert-Maksić
7. Hydrolases – from isolation to function, Marija Abramić
8. Extended π-systems and molecular spectroscopies, Goran Baranović
9. Proton affinity and proton transfer reaction in chemistry, Zvonimir Maksić
10. Germanium, silicon and tin contained polycyclic structures, Davor Margetić

Research and development projects

1. Potential antitumor drugs, Š. Horvat, (MZOŠ, HITRA, TP-B23/2001).
2. Design and synthesis of new beta-agonists based on clenbuterol and terbutaline derivatives, K. Majerski, (TECNA s.r.l. Area di Ricerca, Padriciano, Trieste, Italy).
3. Modelling and Simulation of Protein Folding and the Catalytic Role of Enzymes, subproject under CRO-GRID project. Z. Maksić (MZOŠ - HITRA)

INVITED LECTURES

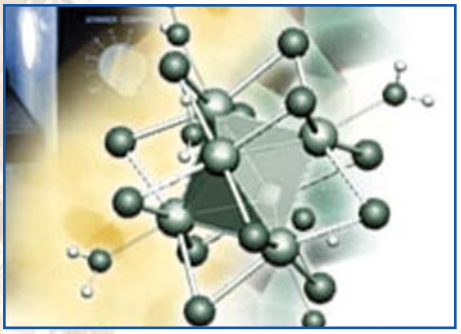
1. M. Eckert-Maksić, “Cycloproparenyl Anions - From Models to Real Systems”, 17th IUPAC Conference on Physical Organic Chemistry, Shanghai, People’s Republic of China, 2004, plenary lecture, August 15-20, 2004.
2. Zvonimir Maksić, “Computational Design of Highly Potent Organic Superbases”, NIC (John von Neumann Institute for Computing) Symposium, Jülich, Germany, February 17-18, 2004.
3. Robert Vianello, “The structure and acidity of 20 α-amino acids”, 2nd Central European Conference - Chemistry Towards Biology, Seggau, Austria, September 26-29, 2004.
4. Mladen Žinić, “Supramolecular Chemistry of Gels” Universite Louis Pasteur de Strasbourg, Faculte de Chimie, Institut Le Bel, May 27, 2004.
5. Mladen Žinić,”Supramolecular Chemistry of Gels-Stereochemistry of Gel Assemblies” Kekule-Institut fuer Organische Chemie and Biochemie, Universitaet Bonn, September 24, 2004.
6. Mladen Žinić, “Supramolecular Chemistry of Gels-Stereochemistry of Gel Assemblies” COST D-31 Organizing Non-Covalent Chemical Systems with Selected Functions, Kick-off Meeting, Prag, November 4 – 7, 2004.

SELECTED PUBLICATIONS

1. Palacios A, Martín F, Mó O, Yáñez M, Maksić ZB. Stable Doubly Charged Positive Molecular Ions Formed by Direct Attachment of Alpha Particles to HCN and HNC. Phys Rev Lett 2004: 92: 133001.
2. Kovačević B, Barić D, Maksić ZB, Müller TH. The Origin of Aromaticity: Important Role of the Sigma Framework in Benzene. Chem Phys Chem 2004: 5: 1352.

3. D'Aleo A, Pozzo J-L, Fages F, Schmuts M, Meiden-Gundert G, Vogtle F, Čaplar V, Žinić M: 11-Aminoundecanoic acid: a versatile unit for the generation of low molecular weight gelators for water and organic solvents. Chem Commun 2004:190.
4. Antol I, Eckert-Maksić M, Lischka H, Maksić ZB. On the Bond-Stretch Isomerism in Benzo[1,2:4,5]dicyclobutadiene System - An Ab Initio MR-AQCC Study. Chem Phys Chem 2004: 5: 975.
5. Abramić M, Šimaga Š, Osmak M, Čičin-Šain L, Vukelić B, Vlahoviček K, Dolovčak L. Highly reactive cysteine residues are part of the substrate binding site of mammalian dipeptidyl peptidases III. Int J Biochem Cell Biol 2004: 36: 434.
6. Leščić I, Zehl M, Müller R, Vukelić B, Abramić M, Pigac J, Allmaier G, Kojić-Prodić B. Structural characterization of extracellular lipase from Streptomyces rimosus: Assignment of disulfide bridges pattern by mass spectrometry. Biol Chem 2004: 385: 1147.
7. Solladié-Cavallo A, Roje M, Welter R, Šunjić V. Two-step Asymmetric Synthesis of Disubstituted N-Tosyl Aziridines Having 98 to 100% ee: Use of a Phosphazene Base. J Org Chem 2004: 69: 1409.
8. Vujasinović I, Veljković J, Mlinarić-Majerski K. New Tin Templates for the Synthesis of Macrocyclic Polythiaether-Polythiaester Ligands. J Org Chem 2004: 69: 8550.
9. Zrinski I, Novak-Coumbassa N, Eckert-Maksić M. Novel Organogermanium Compounds via Metallation of 3-Trimethylsilyl-3-ethoxycarbonylcyclopropene Derivatives. Organometallics 2004: 23: 2806.
10. Piantanida I, Palm BS, Čudić P, Žinić M, Schneider H-J. Interactions of acyclic and cyclic bis-phenanthridinium derivatives with ss- and ds- polynucleotides. Tetrahedron 2004: 60: 6225.
11. Roščić M, Eklund R, Nordmark E-L, Horvat Š, Widmalm G. Stereochemical Assignement of Diastereomeric Imidazolidinone Ring Containing Bicyclic Sugar-Peptide Adducts: NMR Spectroscopy and Molecular Calculations. Eur J Org Chem 2004: 4641.
12. Mlinarić-Majerski K, Veljković J, Kaselj M, Marchand AP. Dihaloadamantanes: Ring Closure versus Rearrangement or Halogen-Displacement Reactions. Eur J Org Chem 2004: 2923.
13. Nemet I, Varga-Defterdarović L, Turk Z. Preparation and Quantification of Methylglyoxal in Human Plasma Using Reversed-Phase High Performance Liquid Chromatography. Clin Biochem 2004: 37: 875.
14. Baranović G, Babić D. Vibrational study of the Fe(phen)2(NCS)2 spin-crossover complex by density-functional calculations. Spectrochimica Acta Part A: Mol Biomolecular Spectroscopy, 2004: 60: 1013.

Division of Materials Chemistry



http://www.irb.hr/en/str/zkm

DIVISIONAL ORGANISATION

Head: Svetozar Musić

The Division of Materials Chemistry (ZKM) consists of the following laboratories:

- Laboratory for synthesis of new materials, Boris Subotić
- Laboratory for precipitation processes, Ljerka Brečević
- Laboratory for radiation chemistry and dosimetry, Dušan Ražem
- Laboratory for solid state chemistry, Želimir Blažina
- Laboratory for complex compounds chemistry, Pavica Planinić
- Group for ichtiopathology – biological materials, Rozelinda Čož-Rakovac

OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is strongly focused on the synthesis of various materials and investigation of their chemical, microstructural and physical properties. We are mainly investigating magnetic and nonmagnetic metal oxides, glass-ceramics, zeolites, cluster compounds, organic polymers, intermetallic compounds and metal hydrides. Members of the group for ichtiopathology-biological materials, recently joined to the division, showed great activities in the application of their research. The radiation chemistry and dosimetry laboratory at the division is the only existing unit in Croatia which has been dealing with all aspects of the physico-chemical effects of ionizing radiations and their applications. The low-dose and high-dose chemical dosimetry systems were developed and internationally accepted. The secondary standard dosimetry laboratory was established. The Division also participated in numerous cooperative activities with different industries, hospitals, state institutions and the University of Zagreb.

TOP ACHIEVEMENTS

Crystallization of zeolite A

The relationship between the concentration of alkali cations and rate of crystal growth of zeolites was studied by (a) measuring the growth rate of zeolite A microcrystals during their crystallization from the systems containing different amounts of Na^+ ions in the liquid phase at constant alkalinity, and (b) defining the relationship between the

Figure 1. Synthesis of zeolite

concentrations of Na, Al and Si in the liquid phase and the crystal growth rate of zeolite A microcrystals. The crystal growth of zeolite A takes place by a surface reaction of aluminate and silicate species around the structure-directing Na^+ ions. The mechanism and the rate of crystal growth of zeolite A were determined. (S. Bosnar et al., Micropor. Mesopor. Mater. 2004: 76: 157).

Figure 2. Thermal analysis of carbonate samples

Model proposing the mode of small inorganic anions in corporation

Based on XRD data, ion chromatography and EPR spectroscopy, the mechanism of incorporation of small inorganic anions into the calcite lattice was proposed. Calcite was chosen as model system, because it was well defined in previous academic studies, and also due to its important role in natural crystallization processes. (J. Kontrec et al., Eur. J. Inorg. Chem. 2004: 4579).

Glass matrix for immobilization of HRLW

The alkali borosilicate matrices for immobilization of highly radioactive liquid wastes (HRLW) were synthesized in our laboratory. Special attention was paid to the admixture of iron, because the radioactive waste contains a significant amount of iron which influences the physical, chemical and microstructural properties of borosilicate matrix. The investigation of synthesized multi-component borosilicate matrices by integral thermally stimulated depolarization current (TSDC) from 170 to 320 K and by windowing polarization showed several relaxation processes which were interpreted and related with the physical, chemical and microstructural properties of borosilicate matrices, including the content of iron. (M. Topić et al., Mater. Chem. Phys. 2004: 87: 311).

Investigations in dosimetry

The thermoluminescent (TL) response of the commercial TLD-700 thermoluminescent dosimeters to 3 MeV protons was analysed as function of dose and particle energy in order to separate the contribution of charged

Figure 3. Radiation dose measurements

particles from the contribution of X-rays to total dose in heavy charged particles irradiations. Thermoluminescent efficiencies of various TL peaks were evaluated relative to gamma ray irradiations, and recommendations for meaningful dosimetry of medical or space heavy charged particle irradiations were made. (S. Miljanić et al., Nucl. Instr. And Meth. In Phys. Res. 2004: A519, 667).

Towards better plastics

The improvement of mechanical properties of polypropylene/polystyrene blends and polypropylene/talc and polypropylene/wollastonite composites modified with EPDM and different styrenic block copolymers was obtained. The mechanical properties of polypropylene/polystyrene blends were optimized by means of compatibility with SEP block copolymer. The impact strength of this ternary blend (PP/PS/SEP) is substantially higher than the corresponding Hivalloy blends (PP/PS/PP-g-PS) (Montell) that currently replace other engineering plastics (polycarbonate, PC/ABS, PC/PBT, ASA, nylon, acetals) in automotive, construction, marine, and consumer applications. (I. Šmit et al. Eur. Polymer J. 2004, 40: 1433).

Figure 4. Work with X-ray powder diffractometer

New alloys for hydrogen storage

New ternary alloys of the general composition $NdNi_{5-x}Ga_x$ ($x \leq 0.5$) were prepared and their interaction with hydrogen was studied. Based on the appropriate thermodynamic properties and the high hydrogen content (about 5 hydrogen atoms per alloy formula unit) the $NdNi_{4.9}Ga_{0.1}$ and $NdNi_{4.8}Ga_{0.2}$ alloys should be regarded as attractive materials for hydrogen storage purposes. (A. Drašner, Ž. Blažina , J. Alloys Comp. 2004: 381: 188)

A new complex of tantalum

The one-step oxidation of the $[Ta_6Cl_{12}]Cl_2 \cdot 6C_2H_5OH$ precursor (that contains the $[Ta_6Cl_{12}]^{2+}$ unit), in the presence of $[(CH_3)_4N]Cl$, using air as an oxidant, provided a direct synthesis of $[(CH_3)_4N]_4[(Ta_6Cl_{12})Cl_6]Cl$ (containing $[Ta_6Cl_{12}]^{3+}$). The crystal structure of the title compound consists of two different types of coordination polyhedra, i.e. four tetrahedral $[(CH_3)_4N]^+$ cations and one octahedral $[(Ta_6Cl_{12})Cl_6]^3$

anion, with one Cl as counter-anion. The presence of three different kinds of Cl atoms [bridging (μ2), terminal and counter-ion] in one molecule makes this substance unique in the chemistry of hexanuclear halide clusters of niobium and tantalum. (M. Vojnović et al., Acta Cryst. 2004: C60: m33).

New method in X-ray powder diffraction

The study of influence of dopands on the structure of materials led to a development of a new method for the estimation of the magnesium fraction in magnesian calcite. The method involves measuring of the X-ray diffraction pattern of magnesian calcite in a narrow 2θ range and individual profile fitting of diffraction lines 113 and 202. The intensity ratio I113/I202 is linearly correlated with Mg fraction. (B. Gržeta et al., in European Powder Diffraction EPDIC8, Eds. Y. Andersson, E. J. Mittemeijer, U. Welzel, Trans Tech. Publications Ltd., Ueticon-Zuerich, 2004, pp. 55-58).

First evaluation of two rapid identification systems ability in fish bacteriology

A new investigation, in which two commercial rapid identification systems (API 20E and BBl Crystal E/NF) were compared in order to reliably identify bacterial isolates from the internal organs of reared sea bass, was performed. The tests yielded different results, suggesting that BBL Crystal E/NF was more reliable in the identification of selected bacteria. However, both systems were found to be applicable for diagnostics of marine fish pathogens, but should be used with caution because of possible misinterpretations. (N. Topić-Popović et al., Vet. Res. Commun. 2004: 28: 93).

PROJECTS

Projects supported by the Ministry of Science, Education and Sport:

1. Research of the crystallization process and use of zeolites, Boris Subotić
2. Kinetics and mechanisms of solid phase precipitation from electrolyte solutions, Ljerka Brečević
3. Synthesis and microstructure of metal oxides and oxide glasses, Svetozar Musić
4. Physico-chemical effects of ionizing radiations, Dušan Ražem
5. Synthesis, characterization and modification of polymers by ionizing radiation, Franjo Ranogajec
6. Intermetallic compounds and metal hydrides, Želimir Blažina
7. Superconducting oxides and polynuclear metal complexes, Nevenka Brničević
8. Influence of dopands on the structure and properties of materials for technical applications, Biserka Gržeta
9. Development of an adaptable technological procedure for the production of precipitated calcium carbonate, Damir Kralj (HITRA TP-01/0098-30)
10. Characterization of the aluminate cement clinker by the Rietveld method, Biserka Gržeta (HITRA TP-01/0098-29).

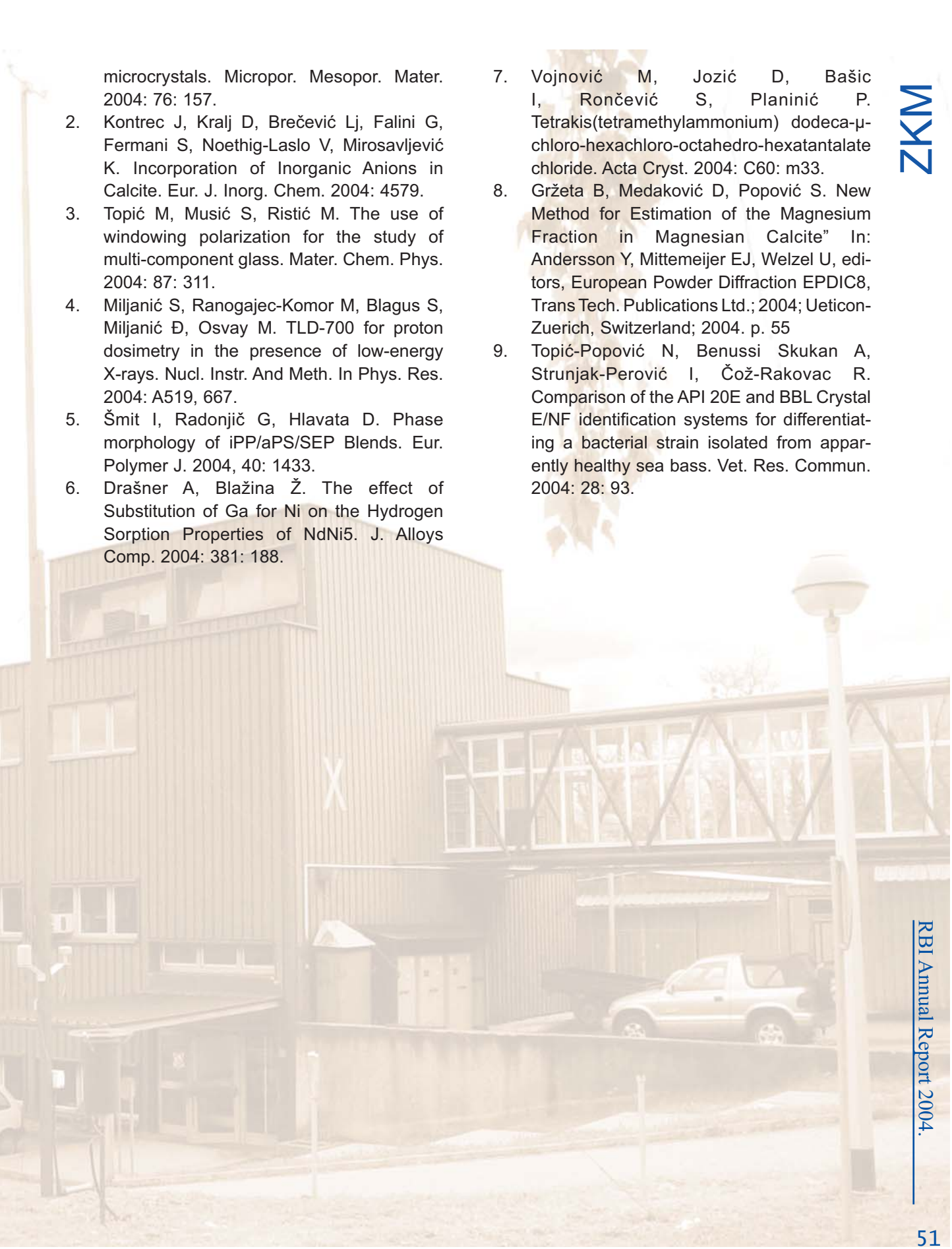
Project supported by the WORLD BANK:

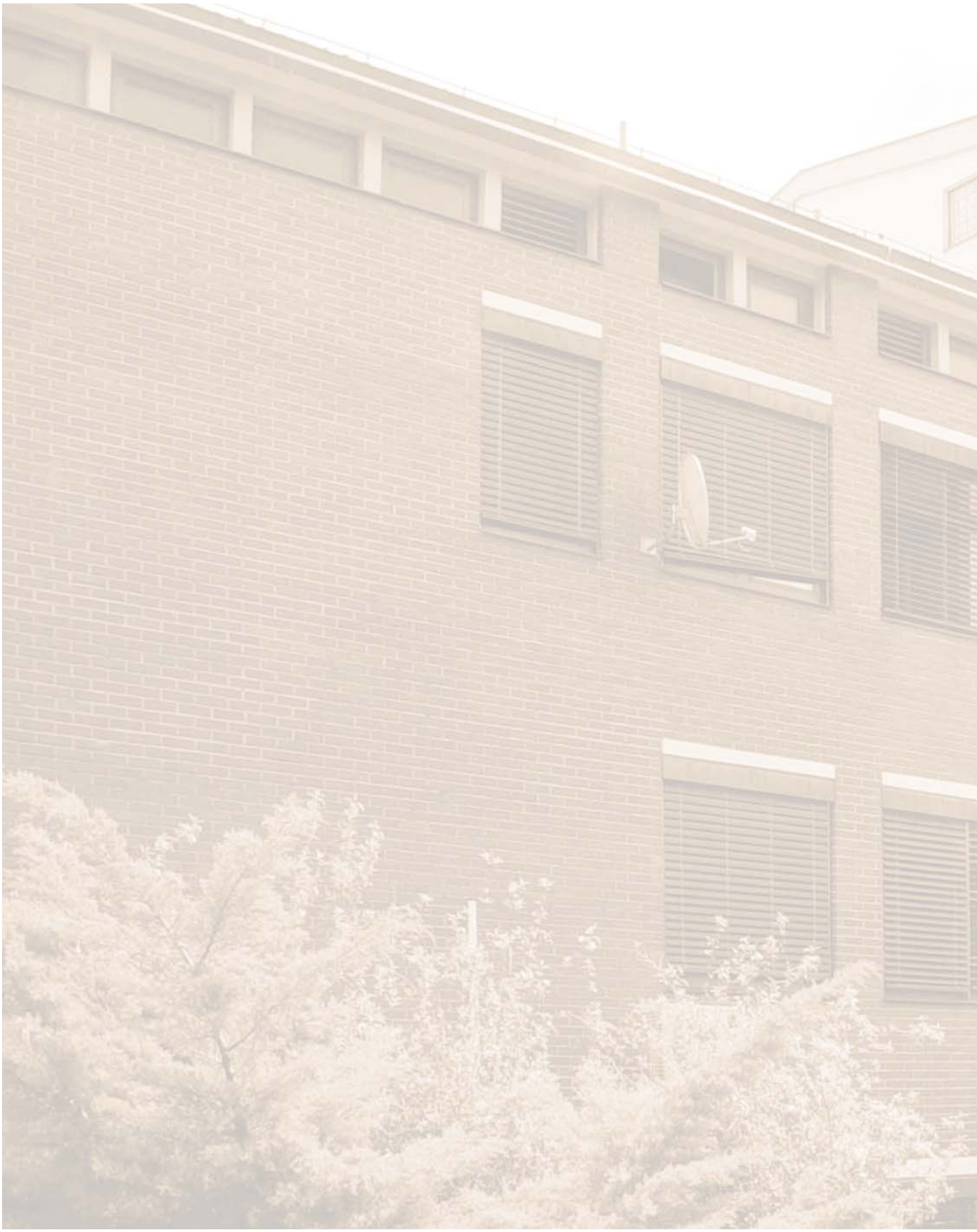
1. Authorized diagnostic center for aquatic organisms diseases, Rozelindra Čož-Rakovac

SELECTED PUBLICATIONS

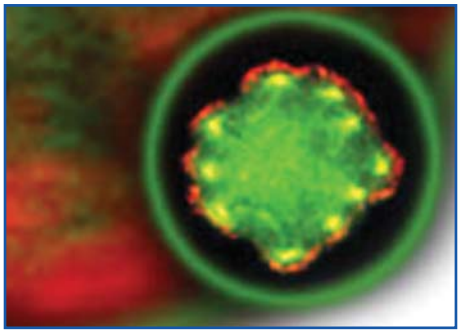
1. Bosnar S, Antonić T, Bronić J, Subotić B. Mechanism and kinetics of the growth of zeolite microcrystals. Part 2: Influence of sodium ions concentration in the liquid phase on the growth kinetics of zeolite A

microcrystals. Micropor. Mesopor. Mater. 2004: 76: 157.
2. Kontrec J, Kralj D, Brečević Lj, Falini G, Fermani S, Noethig-Laslo V, Mirosavljević K. Incorporation of Inorganic Anions in Calcite. Eur. J. Inorg. Chem. 2004: 4579.
3. Topić M, Musić S, Ristić M. The use of windowing polarization for the study of multi-component glass. Mater. Chem. Phys. 2004: 87: 311.
4. Miljanić S, Ranogajec-Komor M, Blagus S, Miljanić Đ, Osvay M. TLD-700 for proton dosimetry in the presence of low-energy X-rays. Nucl. Instr. And Meth. In Phys. Res. 2004: A519, 667.
5. Šmit I, Radonjič G, Hlavata D. Phase morphology of iPP/aPS/SEP Blends. Eur. Polymer J. 2004, 40: 1433.
6. Drašner A, Blažina Ž. The effect of Substitution of Ga for Ni on the Hydrogen Sorption Properties of NdNi5. J. Alloys Comp. 2004: 381: 188.
7. Vojnović M, Jozić D, Bašic I, Rončević S, Planinić P. Tetrakis(tetramethylammonium) dodeca-μ-chloro-hexachloro-octahedro-hexatantalate chloride. Acta Cryst. 2004: C60: m33.
8. Gržeta B, Medaković D, Popović S. New Method for Estimation of the Magnesium Fraction in Magnesian Calcite" In: Andersson Y, Mittemeijer EJ, Welzel U, editors, European Powder Diffraction EPDIC8, Trans Tech. Publications Ltd.; 2004; Ueticon-Zuerich, Switzerland; 2004. p. 55
9. Topić-Popović N, Benussi Skukan A, Strunjak-Perović I, Čož-Rakovac R. Comparison of the API 20E and BBL Crystal E/NF identification systems for differentiating a bacterial strain isolated from apparently healthy sea bass. Vet. Res. Commun. 2004: 28: 93.





Division of Molecular Biology



http://www.irb.hr/en/str/zmb

DIVISIONAL ORGANISATION
Head: Đurđica Ugarković

The Division of Molecular Biology (ZMB) consists of the following laboratories:

- Laboratory of Microbial Genetics, Erika Salaj-Šmic
- Laboratory of Molecular Microbiology, Mirjana Petranović
- Laboratory for Molecular Genetics, Vera Gamulin
- Laboratory for Molecular Genetics of Eukaryotes, Miroslav Plohl
- Gene Regulation Laboratory, Mary Sopta
- Laboratory of Experimental Cancerology, Ivica Rubelj
- Laboratory for Genotoxic Agents, Maja Osmak
- Laboratory for Neurochemistry and Molecular Neurobiology, Branimir Jernej
- Laboratory for Electron Microscopy, Nikola Ljubešić
- Laboratory for Chemical Biology, Volker Magnus
- Laboratory for Biocenotic Investigation, Andrija Željko Lovrić
- Secretary, Marija Kober

OVERVIEW OF THE DIVISION

In 2004, the Division of Molecular Biology made several discoveries related to the mechanisms responsible for drug resistance of human carcinoma cells. The new DNA sequencing service is established within the Department as a central facility for such type of analyses at Ruder Boskovic Institute. Maja Osmak was awarded the Croatian state prize for significant contributions to the development of biological research in Croatia.

TOP ACHEIVEMENTS

Chemotherapy resistance

The increased expression of both, avb3 and coxsackie adenovirus receptor, is responsible for the 5-fold increased adenoviral transduction efficacy in a cell clone resistance to cisplatin. Therefore, it would be very important to determine transduction efficacy of tumors showing cisplatin resistance, because they can be better targets for adenoviral gene therapy than the parental tumor (A. Ambriović-Ristov et al. Int J Cancer 2004: 110: 660).

Understanding the mechanism of chemotherapy

The strong stimulation of SAPK/JNK and p38 kinase, followed by c-Jun/AP-1 activation and Fas-L expression in cisplatin sensitive cells, together with the high DNA damage level, suggests that cisplatin DNA lesions are a major stimulus for the long-term MAP- kinase/AP-1 activation that finally triggers cell death by apoptosis (A. Brozović et al. Int J Cancer 2004: 112: 974).

Figure 1: New ABI PRISM 3100 Avant Genetic Analyser

New DNA service

The first public DNA service in Croatia, offering diverse facilities for DNA analysis to scientists from RBI, the wider academic community and other interested users, was open in December in the presence of Minister Dragan Primorac. For more information, contact the head of the DNA Service, Dr Helena Ćetković.

AWARDS

1. Award to Maja Osmak: The Croatian State Reward, the most prestigeous scientific recognition available in Croatia, was given this year to Maja Osmak, senior research scientist at the Division of Molecular Biology, for research on molecular cell-response to genotoxic stress, and the molecular mechanisms involved in the cell-resistance to genotoxic stress

2. Award to Andreja Ambriović-Ristov: The award of the director of Ruđer Bošković Institute was given this year to Andreja Ambriović-Ristov, associated researcher at the Division of Molecular Biology, for initiating and organizing «Methodological Courses in Biology and Medicine».

PROJECTS

Projects supported by the Ministry of Science, Education and Sport:

1. The role of recombination in DNA repair and genome stability, Erika Salaj-Šmic
2. Regulation of recombination and recombinational repair, Mirjana Petranović
3. Genes and genomes of evolutionary conserved and economically important species, Vera Gamulin
4. Evolutionary dynamics of satellite DNAs, Đurđica Ugarković
5. Organization of heterochromatic DNA sequences in invertebrates, Miroslav Plohl
6. Transcriptional regulation in eukaryotes, Mary Sopta
7. Molecular mechanisms of imortalization and cellular aging, Ivica Rubelj
8. Structure, function and regulation of plasminogen serine proteases, Branko Brdar
9. Cell response to physical, chemical and biological noxa, Maja Osmak
10. Molecular pathophysiology of serotonergic transmission, Branimir Jernej
11. Hydrodynamics of the cerebrospinal fluid, Darko Orešković

12. Structure and function of plastids and cytoskeleton, Nikola Ljubešić
13. Dynamics and genetics of bioactive molecules, Volker Magnus
14. Endemic and relict phytocenoses of Croatia and their mycoflora, Andrija Željko Lovrić

Other projects

1. Biodiversity in Croatia: genetic characterization of autochtonous flora and fauna and economically important species and breeds, Gamulin, V, Tvrtković, N., collaborative project
2. Biological response to damage, Osmak M., claborative project MES (2003-)
3. Usage of telomerase in revitalization of cells and tissues in vitro and in vivo. Rubelj I, collaborative project (2003-)
4. Plant hormones – Physiology, Biochemistry and application. Magnus V, collaborative project (2003-)
5. New potental anti-cancer drugs: diazenes and triazenes (2004-2006) Faculty for Chemistry and Chemical Technology, University of Ljubljana: Mak M. and Polanc S., bilateral collaboration
6. Human adenovirus type 5 retargeted on aminopeptidase (2002-2004) NATO Science Programm, Collaborative linkage grant, Ecole Nationale Vétérinaire d'Alfort, Maisons Alfort, France, Ambriović Ristov A. and Eloit M.
7. Molecular enzymology and enzyme engineering of hydrolases, Vujaklija D., Schwab, H. (Graz University of Technology), bilateral projects
8. Comparative study of distribution, structure and evolution of satellite DNA sequences in the genome of root-knot nematodes in relation with their mode of reproduction. Plohl, M., Castagnone-Sereno, P., Cogito bilateral project

SELECTED PUBLICATIONS

1. Ambriović-Ristov A, Gabrilovac J, Čimbora-Zovko T, Osmak M. Increased adenoviral transduction efficacy in human laryngeal carcinoma cells resistant to cisplatin is associated with increased expression of integrin avb3 and Coxsackie adenovirus receptor. Int J Cancer 2004: 110: 660.
2. Brozović A, Fritz G, Christmann M, Zisowsky J, Jaehde U, Osmak M, Kaina B. Long-term activation of SAPK/JNK, p38 kinase and fas-L expression by cisplatin is attenuated in human carcinoma cells that aquired drug resistance. Int J Cancer 2004: 112: 974.
3. Campanella JJ, Olajide AF, Magnus V, Ludwig-Müller J. A novel auxin conjugate hydrolase from wheat with substrate specificity for longer side-chain auxin amide conjugates. Plant Physiology 2004: 135: 2230.
4. Ćetković H, Muller WE, Gamulin V. Bruton tyrosine kinase-like protein, BtkSD, is present in the marine sponge Suberites domuncula. Genomics 2004: 83: 743.
5. Mravinac B, Plohl M, Ugarković Đ. Conserved patterns in the evolution of Tribolium satellite DNAs. Gene 2004: 332: 169.
6. Csitkovits CV, Đermić D, Zechner LE. Concomitant reconstitution of Tral-catalyzed DNA transferase and DNA helicase activity in vitro. J Biol Chem 2004: 279: 45477.
7. Marais G, Domazet-Lošo T, Tautz D, Charlesworth B. Correlated evolution of synonymous and nonsynonynymous sites in Drosophila. J Mol Evol 2004: 59: 771.

Division of Molecular Medicine

http://www.irb.hr/en/str/zmm

DIVISIONAL ORGANISATION
Head: Krešimir Pavelić

The Division of Molecular Medicine (ZMM) consists of the following laboratories:

- Laboratory of cellular and molecular immunology, Mariastefania Antica
- Laboratory of molecular oncology, Jasminka Pavelić
- Laboratory of molecular pathology, Koraljka Gall-Trošelj
- Laboratory of experimental hematology, immunology and oncology, Jelka Gabrilovac
- Laboratory of biological response modifiers, Tatjana Marotti
- Laboratory of immunochemistry, Biserka Pokrić
- Laboratory of molecular endocrinology and transplantation, Mirko Hadžija
- Laboratory for oxidative stress, Neven Žarković
- Laboratory of molecular neuropharmacology, Danka Peričić
- Laboratory of functional genomics, Marijeta Kralj
- Laboratory of molecular virology and bacteriology, Magdalena Grce

OVERVIEW OF THE DIVISION

The mission of the Division of Molecular Medicine is to expand and strengthen the knowledge of the nature of disease and to develop and improve new strategies for the diagnosis, treatment and prevention of disease. These goals are realized through the evaluation of the impact of genetic factors in disease prevention, the reduction of risk factors, the development and evaluation of new drugs, the exploration of the biochemical and cellular effects of drugs on cells and living organisms, the improvement of scientific methodology, and the education of scientists and students.

The Division is currently developing several strategic projects. These include the development of gene therapy for use against cancer, new methods of diagnosing and deciphering the molecular basis of disease, the refinement of tools based on transcriptomic and proteomic approaches, as well as tissue engineering for the purpose of therapeutic cloning. As such, the Division is emerging as

a pre-eminent centre (centre of excellence), for research in molecular approaches to the study of disease, in south-eastern Europe.

TOP ACHIEVEMENTS IN BASIC RESEARCH

A novel inherited disease of methionine metabolism caused by mutations in the S-adenosylhomocysteine hydrolase gene

Two germ line point mutations in the gene coding for S-adenosylhomocysteine hydrolase were found in a Croatian patient who displayed persistent hypermethioninemia, mild hepatitis, slow psychomotor development, myopathy and signs of mental retardation. This is the first time that mutations in the S-adenosylhomocysteine hydrolase gene have been linked to severe S-adenosylhomocysteine hydrolase deficiency. (I. Baric, O. Vugrek et al. Proc Natl Acad Sci USA 2004: 101: 4234).

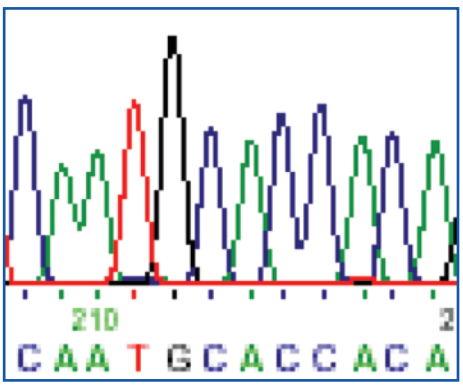


Figure 1A: Mutation for the gene coding for S-adenosylhomocysteine hydrolase

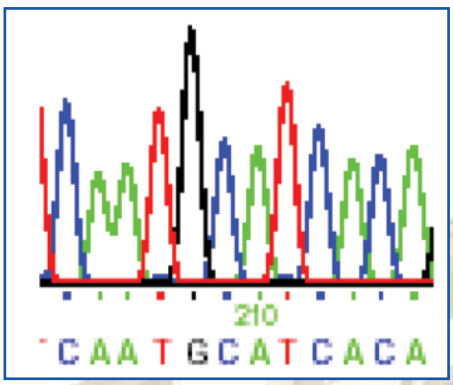


Figure 1B: Control for the gene coding for S-adenosylhomocysteine hydrolase

p73 tumour suppressor in human tumour

Deleted isoforms of p73 (ΔTAp73), a member of p53 gene family, are frequently overexpressed in human cancers and act as a dominative negative inhibitor of wild type p53 and TAp73. However, s stabilization of TAp73 proteins by ΔNp73 (a ΔTAp73 isoform) was found, probably due to the formation of mixed inactive oligomers with TAp73 (N. Slade et al. Cell Death Diff 2004: 11: 357).

Figure 2: The green fluorescence in the nuclei displays nuclear localization of theGFP-Nm23-H1 protein in the pEG-FPC1-nm23-H1 transfected HEp-2 cells arrested in late G1 phase.

Localization of nm23-H1

Green fluorescent protein (GFP)-fused antimetastatic proteins, Nm23-H1 and –H2, display the same localization in transfected cells of head and neck tumours, regardless of their differentiation status (M. Herak Bosnar et al. Exp Cell Res 2004: 298: 275).

The Hedgehog/Patched Signalling Pathway (SHH/PTCH/SMO)

Dermoids, that belong to the developmental cysts and arise from germ cells, were developed as a model for the analysis of the SHH/PTCH/SMO pathway. Malfunctioning of the pathway manifests through the upregulation of a gene PTCH1 and a glioblastoma gene GLI 1. cDNA microarray showed high expression of cyclin D, reflecting the cell cycle.

Embryonic stem cell research

A gene, Oct-4, is a transcription factor which maintains pluripotent phenotype of embryonic stem cells over a long period. By monitoring Oct-4 expression, we tested the ability of embryonic stem cells, derived from 4 mouse strains, to remain pluripotent. Embryonic stem cells of all tested strains have retained Oct-4 expression, in contrast to NOD strain which lost that characteristic. This suggests that rapid downregulation of Oct-4 could be a limiting factor in establishment of NOD embryonic stem cell line.

DPC4 gene mutation in colon and renal cancer

The status of DPC4 tumour suppressor gene in tissues of sporadic colon adenocarcinoma and renal cell carcinoma through loss of heterozygosity analysis and intragenic mutations was detected, thereby displaying a novel somatic mutation (M. Popović-Hadžija et al. Mutation Res 2004: 548: 61).

Ailos, Helios and Ikaros genes in lymphomas

Differential display by PCR, applied on developing lymphocytes, resulted in 15 differentially expressed genes, and the discovery of a new gene for snRNP, expressed by CD4- CD8- lymphocytes. RNA isolation from archival formalin-fixed paraffin-embedded lymph node samples, allowed retrospective gene expression studies on a wide panel of lymphomas. By means of a quantitative PCR (Real time PCR) mRNA in Hodgkin's and Non-Hodgkin's lymphoma patients were analyzed, and a statistically relevant difference in Ikaros family member's expression was found. These findings shed new light on the understanding of transcription factor significance in these diseases. An experimental approach for the identification of regulatory elements associated with the Helios gene was designed.

A novel therapeutic indication

A new approach in the treatment of combat-related posttraumatic stress disorder (PTSD), with psychotic features, has been proposed. A significant improvement in psychotic PTSD was found in patients treated for 3 or 6 weeks with olanzapine or fluphen-

Distribution of aminopeptidase N/CD13 on keratinocytes as compared to distribution on skin fibroblasts.

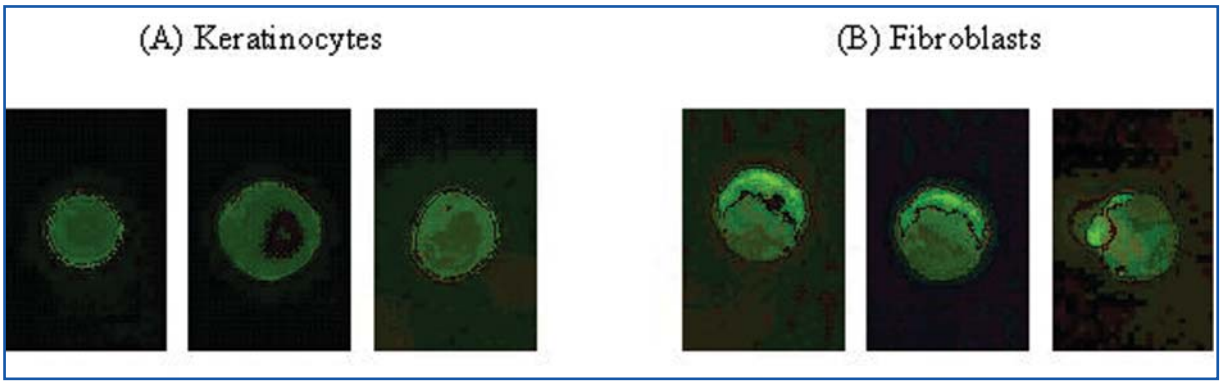


Figure 3: Note moderate, homogenous, ring-like CD13 distribution on keratinocytes (A) versus strong, patchy or polarised CD13 expression on fibroblasts (B).

azine. In addition, olanzapine was shown to be both superior to and more tolerable than fluphenazine in psychotic PTSD patients (N. Pivac et al., Psychopharmacology 2004: 175: 451).

Design of bioactive molecules and new generation of vaccines

A new method for the prediction of α and β protein folding types from RNA, DNA and amino acid sequences was developed. The method enables quick, simple and accurate prediction of α and β protein folds on a personal computer by means of few binary patterns of coded amino acid and nucleotide physicochemical properties. The knowledge about factors responsible for virus virulence, and the role of virus proteins or glycoproteins in the immune response, enabled development of new generations of vaccines based on the antigenic virus subunits.

TOP ACHIEVEMENTS IN APPLIED RESEARCH

Membrane amidopeptidase on human keratinocytes

For the first time evidence has been presented showing that cultured, non-stimulated keratinocytes, obtained from healthy human skin, express membrane aminopeptidase N (EC 3.4.11.2; CD13), associated with enzyme (APN) activity. The role of APN in growth regulation of keratinocytes has been suggested, as inhibitors of APN decrease keratinocyte growth. The role of APN as a co-receptor for adenoviruses has also been studied on several model cell-lines.

Personal molecular medicine and pharmacogenetics

As a part of the research in molecular genetics of colon cancer, a new method for analyzing single nucleotide polymorphisms in was introduced (SNP «real-time» analysis). The prevalence of the four promoter SNPs in TNFα gene, -238, -308, -857 and

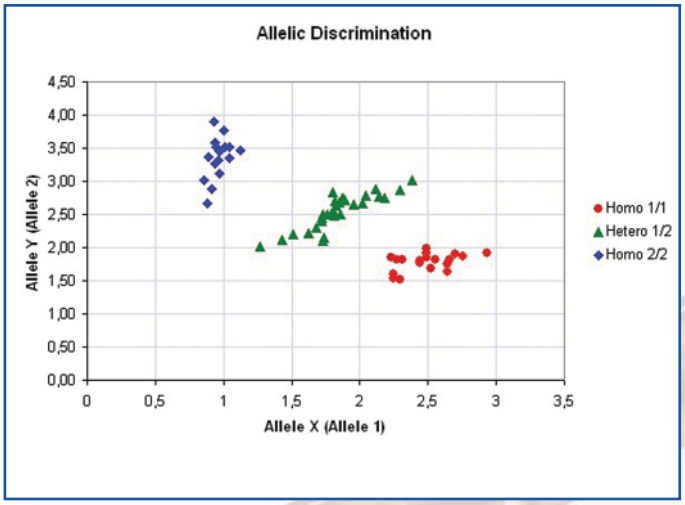


Figure 4: Allelic discrimination -"real-time" SNP analysis

-1031 in the Croatian population and in patients with colon cancer was investigated. "High-production" allele variant -308A was significantly more common in the population with colon cancer than in healthy volunteers. The allelic frequency for three SNPs in the TPMT gene (G238C, G460A and A719G) in the Croatian population was investigated. This type of molecular testing is a molecular determinant of the TMPT activity and is important for optimal drug administration during thiopurines therapy.

A method for analyzing single nucleotide polymorphisms (SNP) for tumour necrosis factor α (TNF α) in gastric biopsies was established. The preliminary results indicate a possible correlation of H. pylori infected patients with the occurrence of gastric lymphoma (Mucosa Associated Lymphatic Tissues, MALT) and carcinoma.

In collaboration with clinical institutions the first pilot study in Croatia on mitochondrial DNA defects in heredodegenerative diseases and diabetes has been finished.

Molecular basis of sexually transmitted infections

Adeno-associated virus type 2 (AAV 2) infection is associated with pregnancy and human papillomavirus (HPV) rather than human cytomegalovirus (HCMV) (M. Grce et al., J Clin Microbiol 2004: 42: 134). HPV infection was strongly associated with a higher grade of cervical intraepithelial neoplasia (CIN), but AAV 2 and HCMV have no impact on CIN. Furthermore, HPV infection could be a cause of miscarriages in human (M. Matovina et al., Fert Steril 2004: 81: 662).

Screening of newly synthesized anticancer compounds

Over 230 newly synthesized compounds were screened in vitro for potential antitumor activity and the possible mecha-

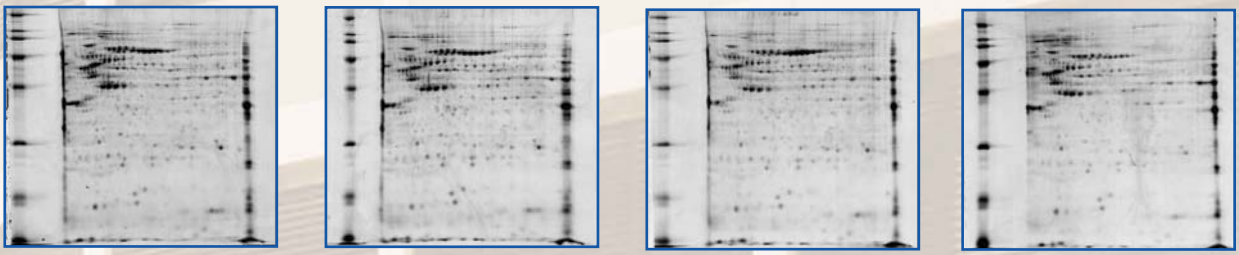


Figure 5: 2DE-gel images of protein samples resolved on IPG strips pH 3-8L. Proteins were visualised with Coomassie staining. Gel images were analysed by the PDQuest software. Differentially expressed proteins were subsequently identified by the MALDI-MS analysis and protein sequencing.

Figure 6: Laminar flow animal protection unit

Figure 7: Experimental mice facility

Figure 8: Breeding unit

nisms of action were ascertained for the most effective ones.

MODERN FACILITIES

Functional Proteomics

Division of molecular medicine has been fully equipped with new 2-D gel electrophoresis instruments and accompanying image analysis software "PDQuest" (Bio-Rad Laboratories, Inc, USA), which have been already successfully introduced into our research practice. This is a first step in establishing proteomic unit in the Division.

New unit for nucleotide sequencing

The unit for nucleotide sequencing on the ABI Prism sequencer has developed, in addition to sequencing, other methods for genetic analyses: SSCP (Single Strand Conformational Polymorphism) and QMP (Quantitative Multiplex PCR), which is generally available to other researchers at the Institute.

New Animal Facility

Renewed and modernly equipped animal quarters were finished, with experimental laboratories within, to meet EU standards for animal units. This unit breeds inbreed strains of mice (BALB/cBkl, CBA/H, C3Hf/Bu, C57BL/Go, C57BL/6-Ly5, NOD) for the research programs. http://www.irb.hr/en/str/zmm/LABS/DLA

EDUCATION

The Division provides over 50 undergraduate and 5 graduate courses annually at Universities in Zagreb, Rijeka and Osijek. Together with Medical Faculty at the University of Zagreb, ZMM continues a joint field of doctoral study in "Molecular Medicine"
(http://bio.mef.hr/docs/Publication.pdf).

PROJECTS

Projects supported by the Ministry of Science, Education and Sport:

1. Molecular mechanisms in the pathogenesis of neuroendocrine tumors, Koraljka Gall-Trošelj
2. Molecular genetics of gastrointestinal tumors, Sanja Kapitanović
3. The SHH/PTCH/SMO signalling pathway in cancer and development, Sonja Levanat
4. Role of FHIT in neuroendocrine tumors, Šime Križanac
5. Insulin-like growth factor family of genes in

lung cancer, Ljubomir Pavelić
6. New therapeutic possibilities in breast cancer, Josip Unušić
7. Genetic and molecular prognostic factors of cervical cancerogenesis, Magdalena Grce
8. Oxidative stress and malignant diseases, Neven Žarković
9. Gene or protein transduction and signalling pathways in transformed cells, Krešimir Pavelić
10. Cxclooxygenase-2: new target for chemoprevention and treatment of colon tumors, Radan Spaventi
11. Molecular mechanisms of immunosuppression, Renata Novak
12. Modulation of immunological response by bioactive peptides, Biserka Pokrić
13. Transcriptional control of lymphocyte development – its role in leukemogenesis, Mariastefania Antica
14. Tumor gene therapy – correction of oncosuppressor genes, Jasminka Pavelić
15. Virus antitumorous action and oncolytic virus vaccine, Mislav Jurin
16. Embryonic cell production of pancreatic-like islets, Mirko Hadžija
17. DNA chip technology in global profiling of tumors, Šime Spaventi
18. Nonlinear modulation of the chronic lymphatic leukemia, Branko Vitale
19. Regulation of ectopeptidases and opioid receptors expression, Jelka Gabrilovac
20. Oxidative/antioxidative status after treatment with opioids/opiates, Tatjana Marotti
21. Neuropharmacology of serotonergic system, Dorotea Mueck-Šeler
22. Neurotransmitters in stress and regulation of GABA-A receptors in vitro, Danka Peričić
23. Assessing functions of the heat repeat in Huntingtin protein, Oliver Vugrek
24. The effects of new drugs and hyperthermia on the growth of mouse tumors and human xenografts, Marko Radačić
25. Immune interactions and immunomodulation in genital herpes infection, Zorka Mikloška

Research and development projects

1. Center for integrative genomics, molecular diagnostics, cellular and gene therapy, Krešimir Pavelić (MZOŠ, JEZGRA, J-1-2004)
2. Development of new analgetic, antirheumatic and antioxidative substances from pine resin, Neven Žarković (MZOŠ, HITRA, TP-01/0098-28)
3. snRNP U2 in lymphoid malignancies, Mariastefania Antica (International Office for Bilateral Cooperation Bonn, Germany)
4. Development a new and improved vaccine against genital herpes, Zorka Mikloška (MZOŠ, HITRA, TP-03/0098-39)
5. Molecular genetic background of Gorlin syndrome, Sonja Levanat (Bilateral Cooperation“Cogito”, Bordeaux, France)
6. The role of the SHH/PTCH/SMO pathway in oncogenesis. Mechanisms of regulation of the SHH/PTCH/SMO pathway in different pathological conditions. (Croatia-Austrian bilateral project 2002-2004), Sonja Levanat, and Annemarie Frischauf (Institute of Genetics and General Biology, University of Salzburg, Austria)

Other projects

1. Ecopropolis - natural antioxidant, Tanja Marotti (BICRO)
2. Nutraceutics for animal use, Tanja Marotti (BICRO)

SELECTED LECTURES

1. Pavelić K.: Nanoporous materials in molecular medicine: cellular and molecular effects. Invited lecture. 3rd Interanational Conference on Mechanisms of Action of Nutraceuticals. Maggie Valley, Waynesville, N.C. USA, 11.-14.11.2004.
2. Pavelić K.: Life Science in the Europe of the Future. Invited lecture. Joint Anniversaries EMBO, EMBC, EMBL. Mannheim, Germany, 15.11.2004.
3. Muck-Šeler, D.: The season of birth and peripheral biochemical markers in psychiatric patients in Croatia. Invited lecture.

European Psychiatry 2004, 19 (suppl 1) 87S, Geneva, Switzerland April 14-18, 2004, 12th AEP (Association of European Psychiatrists) Congress.

4. Žarković N.: Immunodetection of 4-Hydroxynonenal and Other Reactive Aldehydes as Bioactive Markers of Oxidative Stress. Invited lecture. Conference inBerlin (Germany): HNE and Lipid Peroxidation Products: from basic science to medicine, 6.-9.7.2004.
5. Pavelić K.: New developments in molecular oncology. Plenary lecture. 4rd Central European Oncology Congress. Opatija 23.-26.06.2004.

CONFERENCES

1. 4th Dubrovnik Signalling Conference and FEBS Lecture Course on Cellular Signaling, May 21-27,2004, Dubrovnik, Croatia. Organizers: Ruđer Bošković Institute (Krešimir Pavelić), Goethe University Medical School, Frankfurt, Germany (Ivan Đikić) and Yale University School of Medicine, New Haven, CT, USA (Joseph Schlessinger) (Marshall C. and Muller-Esterl W., Mol Cell 2004, 15, 849-852; Lemmon M.A. and Smerdon S.J., Nature Structural & Molecular Biology 2004, 11, 8.)
2. Fourth Croatian Congress of Pharmacology with International Participation, September 15-18, 2004, Split, Croatia. (Organizers: Ruđer Bošković Institute and Croatian Pharmacological Society (Dorotea Mueck-Šeler and Nela Pivac), Satellite Symposium: "Biological markers and pharmacotherapy of psychiatric disorders". (Organizer Nela Pivac).
3. Third International Conference on Mechanisms of Action of Nutraceuticals – ICMAN 3, 12 – 14. November 2004. Haywood County, Western North Carolina, USA. Organizers: North Carolina Biotechnology Center, PhV Corporation and Ruđer Bošković Institute.

SELECTED PUBLICATIONS

Review articles

1. Kraljević S, Mustapić M. Functional Proteomics in Drug Discovery. Screening Trends in Drug Discovery 2004: 5: 10.
2. Kraljević S, Stambrook PJ, Pavelić K. Accelerating drug discovery. EMBO Reports 2004: 5, 837.
3. Moll UM, Slade N. p63 and p73: roles in development and tumor formation. Mol Cancer Res 2004: 2: 371.
4. Levanat S, Musani V, Komar A. The Hedhegog/Patched signaling pathway (SHH/PTCH/SMO) in cancer and development. Period Biol 2004: 106: 217.
5. Pavelić J, Herak-Bosnar M, Kralj M. Gene therapy: concept, current status, moral and ethical aspects. Period Biol 2004: 106: 239.

Additional publications

1. Pivac N, Kozarić-Kovačić D, Muck-Šeler D. Olanzapine versus fluphenazine in an open trial in patients with combat-related posttraumatic stress disorder. Psychopharmacology 2004: 175: 451.
2. Ambriović-Ristov A, Gabrilovac J, Čimbora-Zovko T, Osmak M. Increased adenoviral transduction efficacy in human laryngeal carcinoma cells resistant to cisplatin is associated with increased expression of integrin avb3 and coxsackie adenovirus receptor. Int J Cancer 2004: 110: 660.
3. Herak Bosnar M, de Gunzburg J, Brečević L, Weber I, Pavelić J. Subcellular localization of A and B Nm23/NDPK subunits. Exp Cell Res 2004: 298: 275.
4. Slade N, Zaika AI, Erster S, Moll MU. DeltaNp73 stabilises TAp73 proteins but compromises their function due to inhibitory hetero-oligomer formation. Cell Death Diff 2004: 11: 357.
5. Popović Hadžija M, Radošević S, Kovačević D, Lukač J, Hadžija M, Spaventi R, Pavelić K, Kapitanović S. Status of the DPC4 tumor suppressor gene in sporadic colon carcinoma from Croatian patients: identification

of a novel somatic mutation. Mutation Res 2004: 548: 61.
6. Kapitanović S, Čačev T, Berković M, Popović Hadžija M, Radošević S, Seiwerth S, Spaventi Š, Pavelić K, Spaventi R. nm23-H1 expression and loss of heterozygosity in colon adenocarcinoma. J Clin Pathology 2004: 57: 1312.
7. Barić I, Fumić K, Glenn B, Ćuk M, Schulze A, Finkelstein JD, James SJ, Mejaški-Bošnjak V, Pažanin L, Pogribny IP, Radoš M, Sarnavka V, Scukanec-Špoljar M, Allen RH, Stabler S, Uzelac L, Vugrek O, Wagner C, Zeisel S, Mudd SH. S-adenosylhomocysteine hydrolase deficiency in a human: a genetic disorder of methionine metabolism. Proc Natl Acad Sci USA 2004: 101: 4234.
8. Grce M, Husnjak K, Matovina M, Milutin N, Magdić L, Husnjak O, Pavelić K. Human Papillomavirus, cytomegalovirus and adeno-associated virus 2 infections in pregnant and non-pregnant women with cervical intraepithelial neoplasia. J Clin Microbiol 2004: 42:1341.
9. Matovina M, Husnjak K, Milutin N, Ciglar S, Grce M. Possible role of viral and bacterial infections in miscarriages. Fertil Steril 2004: 81: 662.
10. Kowanetz K, Husnjak K, Holler D, Kowanetz M, Soubezran P, Hirsch D, Schmidt MHH, Pavelić K, De Camilli P, Randazzo PA, Đikić I. CIN85 associates with multiple effectors controlling intracellular trafficking of EGF receptors. Mol Biol Cell 2004: 15: 3155.
11. Cooper E, Hrženjak T, Grdiša M. Alternative sources of fibrinolytic, anticoagulative, antimicrobial and anticancer molecules. Int J Immunopathol Pharmacol 2004: 17: 237.

Chapter in book

1. Slade N, Pavelić J, Pavelić K. Gensko liječenje i kemoprevencija; Gensko liječenje oboljelih od tumora. Internistička onkologija. In: Mršić-Krmpotić Z, Roth A (editor). Zagreb: Medicinska naklada, 2004.

Books

1. Pavelić K. Čuda moderne medicine. Nakladni zavod Globus, Zagreb, 2004.
2. Pavelić K. Wunder der modern Medizin. Nakladni zavod Globus, Zagreb, 2004.

Division of Marine and Environmental Research

http://www.irb.hr/en/str/zimo

DIVISIONAL ORGANISATION
Head: Tarzan Legović

The Division of Marine and Environmental Research (ZIMO) consists of the following laboratories:

- Group for satellite oceanography, Milivoj Kuzmić
- Group for modelling and information systems, Ivica Ružić
- Laboratory for aquatic physical chemistry, Božena Ćosović
- Laboratory for radioecology, Stipe Lulić
- Laboratory for chemistry of trace metals, Goran Kniewald
- Laboratory for electrochemistry and surface chemistry, Dunja Čukman
- Laboratory for molecular ecotoxicology, Tvrtko Smital
- Laboratory for biogeochemistry of organic compounds, Marijan Ahel
- Laboratory for biological effects of metals, Biserka Raspor
- Laboratory for aquaculture and fish pathology, Emin Teskeredžić
- Laboratory for ecological modelling, Vera Žutić

OVERVIEW OF THE DIVISION

During 2004, scientists worked on over 50 research projects contracted by the Ministry of science, sport and education and by outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from satellite oceanography, on the large scale, down to nanotechnology. Each project contributed to the overall mission of the division, which is to strive for excellence in fundamental and applied research of environmental systems, their processes, states and control. The research is directed toward an increase in the knowledge base needed for the optimal management of environment for the benefit of our country and, indeed, the whole world.

In addition, the division scientists coordinated three post-graduate studies, gave 11 undergraduate and 52 post-graduate courses, all at universities in Croatia. The courses were among the select group which obtained the highest marks by students.

TOP ACHIEVEMENTS

Atomic Force Microscopy (AFM) as a tool in marine biophysics

Using the AFM (Figure 1) and a controlled sample preparation method, pioneering images of the 3D structure of a marine gel phase formed episodically in the Adriatic Sea were obtained. The imaging of native marine gel demonstrates that an important fraction of the specimen consists of entangled fibrils. The gel structure exhibits a repeating network of solvent cavities (ranging from 150 to 500 nm) between polymeric strands. The fibrils are rigid macromolecules with typical diameters between 0.6-3 nm and lengths of 0.1-5 μm. An image from the AFM (Figure 2) shows nanoplankton body scale incorporated into gel matrix (2.5 μm x 5 μm, vertical range 20 nm). The sample originates from northern Adriatic marine gel in the summer of 2004.

Highly productive areas in the Mediterraneean

The Gulf of Elefsis, situated in the vicinity of Athens, is a high productivity area regarding the biota. One of the most abundant macro algae existing there is Ulva rigida. The results from the study area showed that U. rigida exudates were a major contributor to the organic ligand pool and contributed considerably to the production of ligands with high metal complexing capacity and/or high surfactant activity. Scoullos M, et al. Marine Chem 2004: 86: 51.)

Figure 1. AFM facility in the Laboratory for ecological modelling.

A new electrochemical method

A novel simple electrochemical method was developed to detect 3d molecular reorientation at the electrode surface. Reorientation of initially flatly adsorbed molecules to slanted or fully erected position on the electrode surface is a common transition during adsorption of organic substances. However, until now the reorientation has not been easily detectable and its occurrence has been often questioned. (Gašparović B, et al. Electroanalytical Chem 2004: 573: 391.)

Fractionation of dissolved organic matter in natural samples using ultrafiltration methodology

The separation of organic matter into different size fractions was examined by using an ultra-filtration procedure. Samples were taken from the North and Middle Adriatic (Šibenik area), as well as in the phytoplankton monoculture Dunaliella tertiolecta. Characterization and determination of sur-

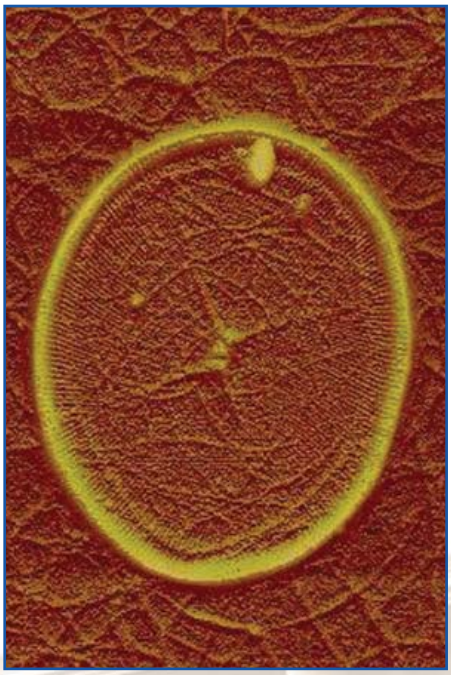


Figure 2. 3D AFM image of nanoplankton body scale in the gel Matrix.

face-active substances in different fractions was carried out by electrochemical methods, accompanied with dissolved organic carbon measurements. The major fraction of organic matter in the natural samples was found in dissolved form (>1 kDa, 76.4% - 87.3%), while the amount of colloid organic matter ranged from 12.7% to 23.6%.

Figure 3. High-Performance Liquid Chromatography-Tandem Mass Spectrometer. (LC/MS/MS, Quantum, Thermo Finnigan) equipped with an accurate mass option.

Manganese in water and sediments of the Krka estuary

A sensitive new method for the determination of manganese on boron-doped diamond electrodes, with ultrasound enhanced accumulation, was employed to determine vertical concentration profiles of manganese in the water column in the vicinity of the former ferromanganese factory (Šibenik Bay, Krka river estuary). The Krka river estuary is highly stratified, with a measured salinity gradient of 200 within half a meter of the freshwater-seawater interface (FSI). An increased concentration of manganese at the FSI was detected, which is a consequence of the accumulation of the organic matter and mineral particles in this layer.

Water-dispersible Amdex-CdSe nanoparticle complexes

Nanoparticle complexes were prepared at room temperature by the rapid mixing of aqueous solutions of either sodium selenide or selenourea with those of cadmium chloride, in the presence of amino-derivatized polysaccharides as a stabilizing agent. These complexes were found to exhibit sufficient luminescence intensity and are thus potential biological labels for multiplexed detection and imaging in medical diagnostics and in molecular and cell biology. (Sondi I, et al. J Colloid Interface Sci 2004: 275: 503.)

The antibacterial activity of nontoxic silver nanoparticles

Silver nanoparticles, which were prepared in a simple and cost-effective manner, were

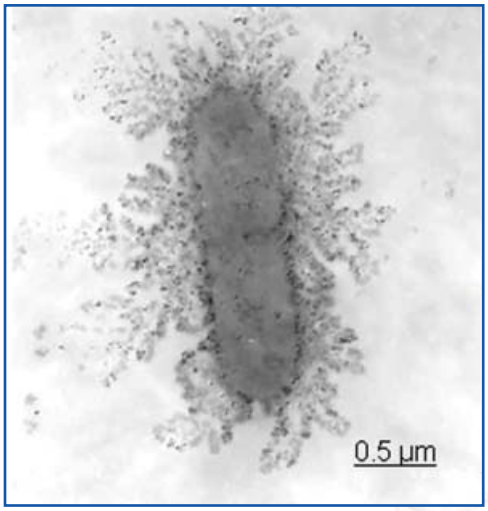


Figure 4. Action of silver nanoparticles against bacteria. Transmission electron micrograph of E. coli cell treated with environmentally friendly silver nanoparticles.

shown to be effective bactericides (Figure 4) against E. coli as a model for Gram-negative bacteria. Such particles therefore are potentially suitable for the formulation of new types of environmentally friendly bactericidal materials. (Sondi I and Salopek-Sondi B. J Colloid Interface Sci 2004: 275: 177.)

Caged mussels Mytilus galloprovincialis

It was found that the variation of digestive gland mass during gametogenesis causes «biological dilution» of metallothionein, a specific biomarker of metal exposure. This fact brings into question the use of this gland as an indicator organ for resolving the impact of metal stress. (Raspor B, et al. Science of the Total Environment 2004: 333: 99.)

Relationship between the MXR defense and cellular detoxification enzymes in fish

A reliable model for research of the relationship between multi- xenobiotic resistence (MXR) defense and phase I. and II. cellular detoxification enzymes was established by using a primary culture of fish (the rainbow trout, Oncorhynchus mykiss) hepatocytes. Furthermore, an effective method for the determination of the environmental presence (in vitro) and effect (in vivo) of hormonally active contaminants, so-called xenoestrogens, in Croatian waters was introduced. The presence of highly potent MXR inhibitors was demonstrated amongst conventional environmental pollutants (pesticides, synthetic musk fragrances, biotransformed crude oil hydrocarbons). (Smital T, et al. Mut. Res. 2004: 552: 101.)

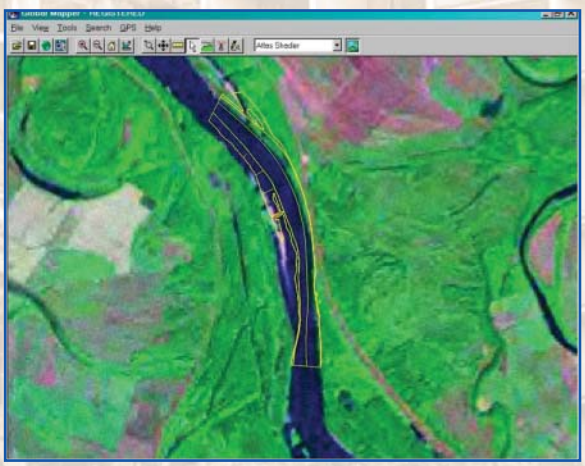


Figure 5. Comparison of the Croatian ENC with a recent satellite picture of the Danube river at the border between Croatia and Hungary.

Development of the Croatian Fairway Information System (CFIS)

Further development of the CFIS was achieved through the creation of the Electronic Navigation Chart (ENC), for the Croatian segment of the Danube river (Figure 5), according to the European Inland ECDIS Standard and WGS-84 compatible coordinate system. This ENC was compared with s recent satellite picture of the same area.

SELECTED INVITED LECTURES

1. Kozarac Z., Certified laboratories in Croatia, National Reference Measurement Infrastructure for Environmental and Food Chemical Measurements in Balkan countries, Plovdiv 04-05. 09.2004
2. Legović T. Effects of submarine outfalls. 4-th European Ecological Modelling Conference, Bled, 28.09.2004.
3. Smital, T., Use of efflux transporters as biomarkers, Hopkins Marine Station, Stanford University, CA, USA, 09.02.2004.
4. Smital, T., Ecotoxicological relevance of MultiXenobiotic Resistance (MXR) defense system in aquatic organisms, Bodega Bay Marine Laboratory. University of California Davis, Davis, CA, 03.04.2004.
5. Sondi, I., A critical review of the electrokinetics of clay mineral particles. 2nd European Clay Conference. Miskolc, Hungary, September 20-24, 2004.
6. Sondi I., Homogeneous precipitation of calcium carbonate polymorphs by enzyme catalyzed reactions. 2nd International Aegean Physical Chemistry Days.Ayvalik/Balikesir, Turkey, October, 7-10, 2004.

ORGANIZED CONFERENCES

Biogeochemical Processes in Anoxic Marine Environments, Croatian-British Workshop, Zagreb, January, 17- 20. 2004 (I. Ciglenečki - Jušić)

PROJECTS

Projects supported by the Ministry of Science, Education and Sport:

1. Tidal and longer-period dynamics of the northern Adriatic, Milivoj Kuzmić
2. Analysis and biogeochemistry of organic compounds in the aquatic environment, Marijan Ahel
3. Physical chemistry and biogeochemistry of trace metals in aquatic systems, Ivanka Pizeta
4. Nature and reactivity of organic substances in marine and environment, Božena Ćosović
5. Electroanalytical research in liquid and solid electrolytes, Milivoj Lovrić
6. Models and info. systems for environmental protection and navigation management, Ivica Ružić
7. Protection of biocoenotic balance in aquaculture receiving waters, Emin Teskeredžić
8. Preparation and properties of metal surfaces in the environmental protection, Dunja Čukman
9. Interfacial processes and eutrophication, Vera Žutić
10. Radionuclides in environmental systems, Delko Barišić
11. Metals and cellular biomarkers, Biserka Raspor
12. Persistent organohalogen pollutants in some coastal area of Dalmatia, Mladen Picer
13. Geochemistry of recent and ancient sedimentary systems of the Adriatic platform, Goran Kniewald
14. Modelling aquatic ecosystems, Tarzan Legović
15. Microbial communities as catalysts in biotransformation processes, Dubravka Hršak
16. Multixenobiotic resistance mechanism as a biomarker of environmental quality, Tvrtko Smital

Selected research and development projects

1. Treatment of wastewaters using membrane techniques (HITRA), Ivan Mijatović and Marijan Ahel
2. Conceptual model for biological treatment of effluents from atrazine production (HITRA), Dubravka Hršak
3. Development of new type of electrochemical sensor and measurement system for reactive microparticles (HITRA), Vera Žutić
4. Nano-systems and nano-tecnology (The role of enzymes in the formation of inorganic colloids), Croatia-Slovenia Collaboration Project, Ivan Sondi
5. Reduction of environmental risks and health risks, posed by Emerging Contaminants, through advanced treatment of municipal and industrial wastes, EMCO (EU-FP6), Marijan Ahel
6. Reference laboratory. Ministry of Agriculture, Forestry and Water Management, Water Management Directorate, Božena Ćosović, Zlatica Kozarac, Dubravka Hršak, Biserka Raspor
7. Sava River Basin: Sustainable Use, management and Protection of Resources. EU FP6, INCO-CT-Biserka Raspor (WP3 Coordinator)
8. Environmental sono-electroanalysis: manganese speciation and determination, The Royal Society, Šebojka Komorsky-Lovrić and R. Compton (Oxford University).
9. Monitoring of Dunav water quality, Croatian Water Management, Stipe Lulić
10. Radiological monitoring around Krško, Nuclear Power Plant Krško, Slovenija, Stipe Lulić
11. Assessment of selected POPS in the atmosphere and water ecosystems from waste materials generated by warfare in the area of former Yugoslavia (APOPSBAL), Mladen Picer
12. MONALISA, The role of natural organic matter in speciation of bioavailable contaminants in coastal waters, French-Croatian Cooperation, Goran Kniewald
13. Mediterranean Mussel Watch Program. International project led by the International Commission for the Scientific Exploration of the Mediterranean Sea (CIESM), 2002 – 2006,
    Goran Kniewald and Delko Barišić (Coordinators in Croatia)
14. Mechanism of mucilage formation in the Northern Adriatic Sea, Bilateral Cooperation project with NSF, USA, Scripps Institution of Oceanography, UCSD, Vera Žutić
15. Ecosystem Approach for Sustainable Aquaculture, ECASA (EU-FP6) Tarzan Legović
16. Croatian national monitoring programme, Božena Ćosović et al.
17. An integrated environmental monitoring system for Croatian freshwater, estuarine and coastal marine areas. Croatian-Norwegian International project, Biserka Raspor, Smiljana Britvić, Goran Klobučar
18. Environmental impact assessment study of fish and shellfish culture in Krka estuary, Emin Teskeredžić (Coordinator)
19. Environmental impact assessment study of fish and shellfish culture in Kaldonta bay (Island
    Lošinj), Emin Teskeredžić (Coordinator)
20. Monitoring of environment and fish culture in Kaldonta bay, Emin Teskeredžić (Coordinator)
21. Data analysis for the needs of the Morinje Bay ecological study, Goran Mihelčić
22. Assessment of current radioecological conditions. Marina Kaštela, Delko Barišić
23. Geochemistry of ecotoxic metals in NP Krka, Neven Cukrov
24. Determination of ecotoxic metals in water and sediments of NP Mljet, Vlado Cuculić
25. Determination and speciation of metals in aquatic sediments and porewaters, French-Croatian bilateral COGITO project, Nevenka Mikac (Coordinator)
26. Mitigation of environmental consequences of the war in Croatia – risk assessment of hazardous chemical contamination, Norwegian-Croatian joint project,
    Marijan Ahel and Goran Kniewald (Coordinators)
27. Ecosystem dynamics, marine chemistry, aquaculture and coastal management in

the Adriatic and North Norwegian coastal zone, Norwegian Cooperation Programme with South East Europe, Božena Ćosović (Croatian coordinator)

28. Electrochemical studies of sea-surface microlayers, ALIS, British Council and Ministry
of Science, Sport and Education, Zlatica Kozarac (Croatian coordinator)
29. Development of an international standard of data warehouse for Danube waterway, Ministry
of sea, tourism, transport and development, INTERREG III B CADSES cooperation, Ivica Ružić
30. Adriatic as a particularly sensitive sea area, Tarzan Legović (Coordinator)

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1. Gašparović B, Risović D, Ćosović B. The simple electrochemical method for detection of 3d molecular reorientation in adsorbed layer of organic substances. Journal of Electroanalytical Chemistry 2004: 573: 391.
2. Grahek Ž, Rožmarić Mačefat M. Isolation of iron and strontium from liquid samples and determination of 55Fe and 89, 90Sr in liquid radioactive waste. Analytica Chimica Acta 2004: 511: 339.
3. Horvat-Radošević V, Kvastek K. Hydrogen/Anion Electrosorption at Rhodized Electrodes as Revealed by Electrochemical Impedance Spectroscopy. Journal of Electroanalytical Chemistry 2004: 566: 451.
4. Komorsky-Lovrić Š, Mirčeski V, Kabbe C, Scholz F. An In Situ Microscopic Spectroelectrochemical Study of a Three-Phase Electrode where an Ion Transfer at the Water Nitrobenzene Interface is Coupled to an Electron Transfer at the Nitrobenzene Graphite Interface. Journal of Electroanalytical Chemistry. 2004: 566: 371.
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9. Raspor B, Dragun Z, Erk M, Ivanković D, Pavičić J. Is the digestive gland of Mytilus galloprovincialis a tissue of choice for estimating cadmium exposure by means of metallothioneins? Science of the Total Environment 2004: 333: 99.
10. Scoullos M, Plavšić M, Karavoltsos S. Speciation studies of copper in the Gulf of Elefsis: The role of macroalgae Ulva rigida. Marine Chemistry 2004: 86: 51.
11. Smital T, Luckenbach T, Sauerborn R, Hamdoun MA, Vega LR, Epel D. Emerging contaminants - pesticides, PPCPs, microbial degradation products and natural subst ances as inhibitors of multixenobiotic defense in aquatic organisms. Mut. Res. 2004: 552: 101.
12. Sondi I, Salopek-Sondi B. Silver nanoparticles as antimicrobial agent: a case study on E.coli as a model for Gram-negative bacteria. J. Colloid. Interface Sci. 2004: 275: 177.
13. Sondi I, Siiman O, Matijević E. Synthesis of CdSe nanoparticles in the presence of aminodextran as stabilizing and capping agent. J. Colloid. Interface Sci. 2004: 275: 503.

Center for Marine Research

http://www.irb.hr/en/str/cim

DEPARTMENT ORGANISATION
Head: Nenad Smodlaka

The Center for Marine Research (CIM) consists of the following laboratories:

- Laboratory for ecology and systematics, Ana Travizi
- Laboratory for processes in the marine ecosystem, Danilo Degobbis
- Laboratory for marine molecular toxicology, Renato Batel
- Laboratory for ecotoxicology, Bartolo Ozretić

OVERVIEW OF THE DEPARTMENT

The Ruđer Bošković Institute, and in particular its Center for Marine Research (CMR), is responsible for coordinating the national monitoring and research project "Jadran". As a direct result of this project, the level of collaboration among all national institutions dealing with marine research, including groups from universities, has been significantly enhanced. The collected data are used to fulfil Croatia's international obligations derived from various ratified documents concerning environmental protection. Moreover, the project represents a wider regional initiative, recommended by the Croatian-Italian-Slovenian trilateral commission for the protection of the Adriatic, to establish a common observing system (Coordinated Adriatic Observing System - CAOS). It is expected that this observing system will become a permanent fixture suitable for future marine research in the Adriatic. International projects such as ADRICOSM (2002-2005) and future Interreg projects (Requisite and Adriamet scheduled in 2005) are closely linked to "Jadran" project.

In addition to the regular activities required in the framework of the "Jadran" project, efforts were made by CMR scientists towards detailed monitoring of the mucilage event (June-July) and of the spreading of the dangerous jellyfish Pelagia noctiluca (Figure 1) during 2004. This species last invaded the Adriatic in the late seventies and early eighties.

Figure 1. Jellyfish Pelagia noctiluca in the Rovinj harbor – 11 October 2004.

freshened waters, formed off the Po River delta, even in conditions of extremely high freshwater discharge rates. This is important for the ecosystem of the north-eastern Adriatic as it is highly sensitive to the amounts of freshened water received. For example, in conditions of increased freshwater input, the decomposition of sedimented organic matter, produced in intense algal blooms, can cause serious oxygen depletion in the bottom layer with mass mortality of benthic organisms.

TOP ACHIEVEMENTS

Influence of circulation on undesirable events in the northern Adriatic

Mucilage and hypoxia events in the northern Adriatic were observed to occur in closed circulation cells, containing freshened water. These events were found to persist in such areas for the long time periods (up to several months). The north-eastern wind ("bura") blowing limited the eastward spreading of

Mucilage event mechanisms

TEP as a mucilage precursor

The levels of accumulated TEP (transparent exopolymer particles; Figure 2) were found to undergo an abrupt decrease in association with mucilage formation. In addition to this clearly significant factor in the northern Adriatic mucilage phenomenon, the imbalance in the "microbial loop" further characterised the event. Marine bacteria isolated from water and mucilage were found to

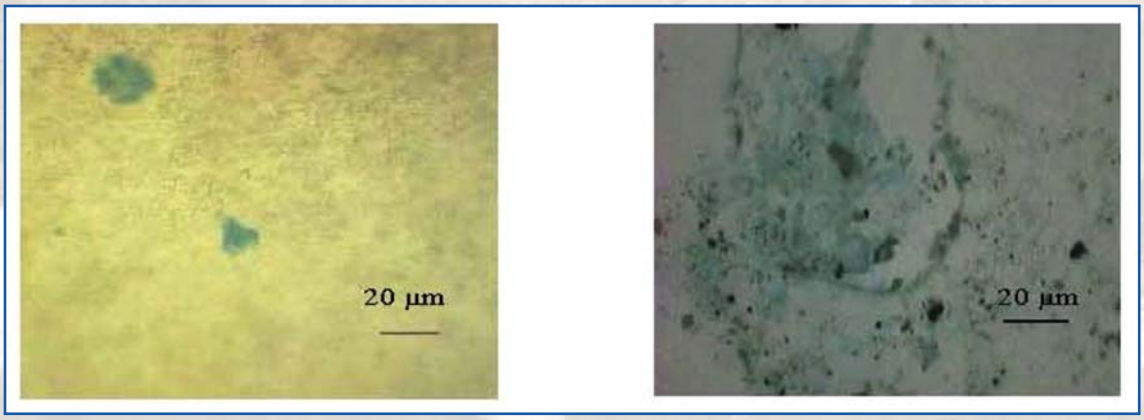

Figure 2. Usually recognizable TEP and accumulated TEP-like matter.

possess potential for TEP production.

Bacterial community fatty acid profiles

The fatty acid profiles of the bacterial community were established as useful discriminating parameters in the evaluation of the mucilaginous aggregate age and degradation phase. During the aggregate aging process, degradation of mucous matrix, bacterial succession and phytoplankton growth took place inside the aggregates.

Figure 3. The alien macroalgae Caulerpa racemosa in the Vrsar area – 26 August 2004.

Benthic faunal communities

The study of long-term changes of macrophytobenthos in the Rovinj coastal zone (western Istria) showed significant differences in the community structure between polluted and pristine localities.

A seasonal study in the offshore area of the north-eastern Adriatic revealed rich and diverse benthic meio- and macrofauna dominated by Nematoda, Polychaeta and Bivalvia. A considerable portion of the sensitive taxa (Copepoda, Echinodermata) reflected a stable community structure, characteristic of quite favourable environmental conditions in a benthic subsystem.

Alien macroalgae

The alien green algae Caulerpa racemosa (Figure 3) invaded the Vrsar coastal area (western Istria). To date, this tropical species was reported only in the central and southern Adriatic Sea.

Seasonal adaptation

Fatty acid composition of Caulerpa taxifolia (M. Vahl.) revealed that stimulation of growth and spreading could be explained by a successful adaptation to the seasonality of environmental parameters (primarily temperature).

Tributyltin effect on organisms

A high level of imposex degree (genital disorder registered in the females of Hexaplex trunculus snails) and high tributyltin (TBT) levels in the snail's soft tissue indicated that remarkable TBT pollution occurs in some northern Adriatic harbour areas.

The extreme toxicity of TBT prevented normal shell biomineralisation of the European flat oyster Ostrea edulis (Linnaeus) from the Rovinj marina (western Istria; Figure 4). The red circles on both O. edulis valves indicate anomalies of the inner nacreous shell layer that consisted of stacked "cham-

Figure 4. Ostrea edulis (Linnaeus) shells exposed to TBT.

bers“ filled with a gelatinous substance. A significant tin content was detected only in the newly formed “chambers”.

Stress-70 proteins in the marine mussel Mytilus galloprovincialis as biomarkers of environmental pollution: a field study

The levels of stress-70 proteins in the gills of the mussel Mytilus galloprovincialis from different sites of the Rovinj coastal area (northern Adriatic, Croatia) were analysed. Two bands of stress-70 proteins (HSP70 and HSP72, pI 5.7-5.9 and 5.5-5.6, respectively) were constitutively present during the year in all of the samples. Maximal levels of stress-70 proteins were observed in mussels in late summer (September) and minimal levels in early winter (December). Significant differences in HSP70 and HSP72 contents were detected in mussels from the unpolluted control site, compared to mussels from sites with urban and industrial pollution. Only HSP70 content showed a significant correlation with the sea temperature ($r=+0.822$, $p<0.05$), while other differences in HSP72 levels may be attributed to the pollution mediated effects.

Influence of herbicide, 2, 4-dichlorophenoxy acetic acid, on haemocyte DNA of in vivo treated mussels

The influence of the herbicide 2,4-dichlorophenoxy acetic acid (2,4-D) on the haemocyte DNA of in vivo treated mussels Mytilus galloprovincialis has been investigated by flow cytometry and epifluorescence microscopy. Haemocyte proliferation and atypical flow cytometric DNA histograms were observed in mussels treated with 20 and 100 μg/g of 2,4-D. The stimulation of proliferation by 2,4-D was also obvious by DNA labelling with BrdU followed by FITC conjugated anti-BrdU MoAb visualised by epifluorescence micros-

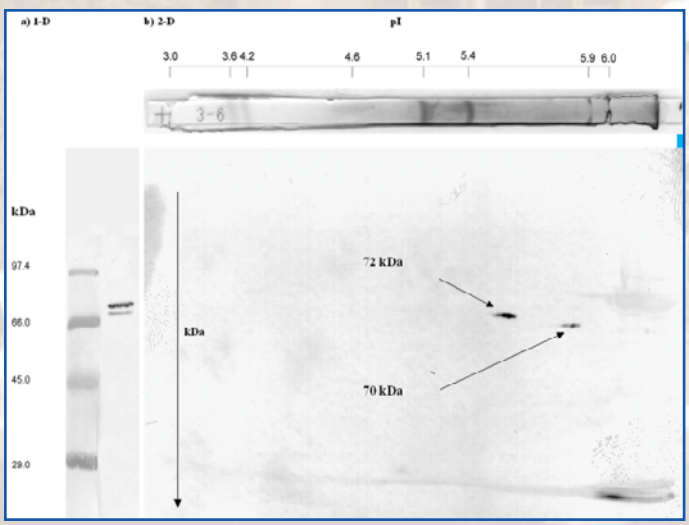

Figure 5. Western blot analysis of stress-70 proteins in mussel gills separated with a) 1-D and b) 2-D gel electrophoresis. Two isoforms of stress-70 proteins, HSP70 (pI 5.7-5.9) and HSP72 (pI 5.5-5.6) were detected using a monoclonal antibody against bovine HSP70 (Clone BRM-22, Sigma).

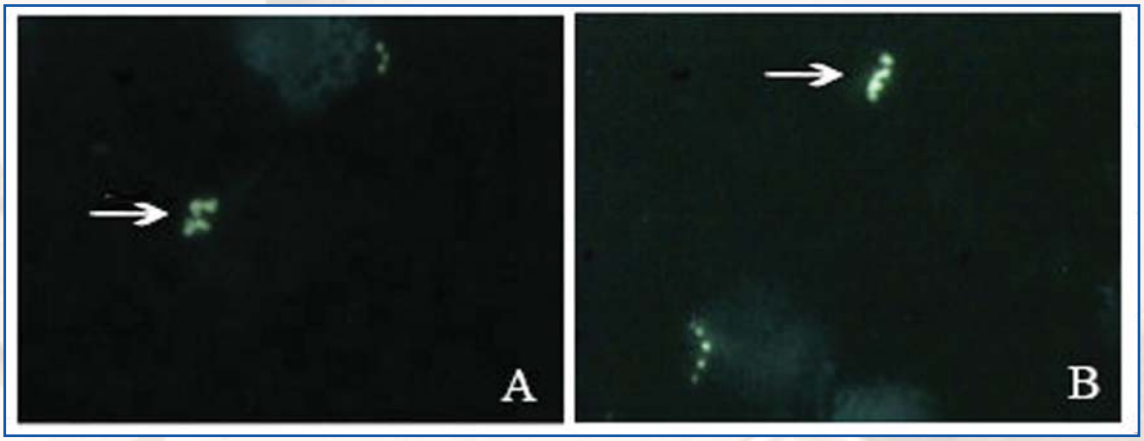

Figure 6. Sister chromatide exchange (SCE) in haemocytes obtained from 48 h of in vivo 100 µ/g 2,4-dichlorophenoxy acetic acid treated mussels M. galloprovincialis. SCE counts (arrows) were performed in 10 metaphases in each one of the 20 treated mussels. Fluorescence photomicrographs were obtained with DAPI counterstained haemocytes illustrating BrdU incorporating cells followed by FITC-conjugated anti-BrdU antibody with colchicines observed under UV light on a Nicon Microphot-FXA/SA epifluorescence microscope.

copy. An apoptotic sub-G(0) peak resulted in mussels that were exposed to higher doses of herbicide at 100 and 500 µg/g as well as a subpopulation that could be detected by flow cytometric analysis. In these experiments evidence of morphological changes characteristic for apoptotic cells was sought by fluorescence microscopy. A low percentage of cells in S as well as in G(2)M phase, indicating G(1), arrest were detected in haemocytes from those mussels that had survived 4 days of 20 mug/g 2,4-D exposure. In addition, sister-chromatid exchanges (SCE) could be seen with the immumolabelling BrdU method. Thus, in vivo treatment and the subsequent uptake of 2,4-D causes serious genetic consequences and raises concerns regarding the potential overall fitness and health effects in mussel populations.

SELECTED INVITED LECTURES

1. Medaković D. Influence of different pollutants on the Adriatic ecosystem. Croatian Geographycal Society and Faculty of Philosophy, Zadar, 25 May 2004.
2. Medaković D. Influence of different pollutants on the Adriatic ecosystem. Hempel, Umag, 10 June 2004.
3. Medaković D. Influence of different pollutants on the Adriatic ecosystem. Annual meting of the Istrian Geographical Society, 10 December 2004.

PROJECTS

Basic research projects supported by the Ministry of Science, Education and Sport:

1. Mechanism of long-term changes in the Adriatic Sea ecosystem, Danilo Degobbis
   Programmed biosynthesis and genotoxic risk assessments, Renato Batel
2. Physiological and biochemical indicators of toxicological stress in marine biota, Bartolo Ozretić
3. Ecophysiological studies and stress response in marine organisms, Čedomil Lucu

4. Systematic research of the Adriatic Sea as a base for sustainable development of the Republic of Croatia (Project «Adriatic»), Croatian national monitoring programme, Nenad Smodlaka

Other projects

1. Biomineralisation and oxygen and carbon isotope composition in the shells of several freshwater and land snail species dependant on environmental conditions, Davorin Medaković (bilateral collaboration with Slovenia)
2. Enzymatic activity of Carbonic Anhydrase and Biomineralisation Processes in Barnacles, Davorin Medaković (CNR, Italy-NATO Research Programme)
3. Biomonitoring of environmental contamination by TBT on Mediterranean coasts, Davorin Medaković (NATO Science Programme)
4. Changes of biomineralisation processes, mineral and stable isotope compositions in bivalvia shells from the Adriatic Sea caused by pollution, Davorin Medaković (bilateral collaboration with Slovenia)
5. Regional collaboration in environmental monitoring and forecasting in the northern Adriatic Sea, Nenad Smodlaka (quadrilateral collaboration with U.S.A., Italy and Slovenia)
6. Adriatic Sea integrated coastal areas and river basin management system pilot project (ADRICOSM), Nenad Smodlaka (quadrilateral collaboration with Italy, France and Slovenia)
7. Molekulare Biotechnologie und Wirkstoffe mariner Schwaemme sowie Schwamm-assoziierter Mikroorganismen (Biotec-Marin), Project: Schwaemme aus Rovinj (Kroatien) – Extractbereitstellung und Marikultur, Renato Batel (bilateral collaboration with Germany)
8. Biosensor methods for the assessment of the effects pollution, Renato Batel (bilateral collaboration with Germany)
9. Quantitative determination p53 mRNA expression in different tissues of the mussel Mytilus galloprovincialis, Milena Mičić (bilateral collaboration with Slovenia)
10. Mechanism of mucilage formation in the northern Adriatic Sea: A component of CREICO (Cooperative research on ecological interactions in the coastal ocean, NSF), Vera Žutić (quadrilateral collaboration with U.S.A., Italy and Slovenia)

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1. Bihari N, Fafanđel M. Interspecies differences in DNA single strand breaks caused by benzo(a=pyrene and marine environment. Mutat Res 2004: 552: 209.
2. Bihari N, Mičić M, Fafanđel M. Seawater quality along the Adriatic coast, Croatia, based on toxicity data. Env Toxicol 2004: 19: 109.
3. Cozzi S, Ivančić I, Catalano G, Đakovac T, Degobbis D. Dynamics of the oceanographic properties during mucilage appearance in the northern Adriatic Sea: analysis of the 1997 event in comparison to earlier events. J Mar Syst 2004: 50: 223.
4. Gržeta B, Medaković D, Popović S. New method for the estimation of magnesium fraction in magnesian calcite. In: Andersson Y., Mittermeijer E.J., Welzel U. (Eds). European Powder Diffraction EPDIC 8. Materials Science Forum. Trans Tech Publications Inc.Uetikon-Zürich, 2004, Vols. 443-444, pp.55-58.
5. Hamer B, Pavičić-Hamer D, Müller WEG, Batel R. Stress-70 proteins in marine mussel Mytilus galloprovincialis as biomarkers of environmental pollution: a field study. Environment Int 2004: 30: 873.
6. Iveša Lj, Blažina M, Najdek M. Seasonal variations in fatty acid composition of Caulerpa taxifolia (M. Vahl.) C. Ag. in the northern Adriatic Sea (Malinska, Croatia). Bot Mar 2004: 47: 209.
7. Mičić M, Bihari N, Mlinarič-Raščan I. Influence of herbicide, 2, 4-dichlorophenoxy acetic acid, on haemocyte DNA of in vivo treated mussel. J Exp Mar Biol Ecol 2004: 311: 157.

8. Morović M, Precali R. Comparison of satellite colour data to in situ chlorophyll measurements. Int J Remote Sensing 2004: 25: 1507.
9. Supić N, Grbić B, Vilibić I, Ivančić I. Long-term changes in hydrographic conditions in northern Adriatic and its relationship to hydrological and atmospheric processes. Ann Geophys 2004: 22: 733.
10. Travizi A, Zavodnik N. Phenology of Caulerpa taxifolia and temporal dynamics of its epibionthic meiofaunain in the port of Malinska (Croatia, northern Adriatic Sea). Sci Mar 2004: 68: 145.
11. Vilibić I, Supić N. Dense-water generation episodes in the Northern Adriatic, Nuovo Cimento 2004: 27: 47.
12. Vilibić I, Grbec B, Supić N. Dense water generation in the north Adriatic in 1999 and its recirculation along the Jabuka Pit, Deep Sea Res 2004: 51: 1457.

Center for Informatics and Computing

http://www.irb.hr/cir

ORGANISATION OF THE CENTER
Head: Karolj Skala

The Center for Informatics and Computing (CIR) consists of the following sections:

- The optoelectronics and hypermedia laboratory, Karolj Skala
- Information and Computer Technology research and development, Zorislav Šojat
- Information systems, Neven Kmetić
- Service and maintenance, Ratko Mileta

OVERVIEW OF THE CENTER

Grid research and application

In 2004, CIR began the e-Science program realisation based on the **ICST** (Information Communication Science Technology) at Grid platforms. Started with the National Grid Initiative poly-project CRO-GRID with 11 institutions and over 50 explorers. The goal of the project is the establishment of a national computing grid. CIR is the leader of the CRO-GRID Applications project and member of the CRO-GRID Infrastructure project. CIR is also developing a Grid Portal through which scientists will be able to access the grid computing resources and submit complex compute-intensive jobs.

A second important realisation of CIR in 2004 was the successful application for the EU FP6 project SEE-GRID, which started in May, [Fig 1]. In the remaining seven months of the project execution during 2004, some important results were achieved. Specifically, a test grid was established between Zagreb (RBI) and Budapest (MTA SZTAKI). It is intended to acquire CERN certification for this grid and further that it become established as a permanent participant in the EGEE e-Science programme. Finally, in 2004 RBI/CIR was elected to be the main site for the SEE-GRID VOMS (Virtual Organisation Membership Service) server.

Information system development and service

The service and maintenance departments installed a new monitoring service based on Open-Source application (Linux OS) called Nagios. This service is capable of discovering network problems and establishing administrative contacts in a variety of different ways (email, instant message,

SMS, phone call). Current status information, historical logs, and reports can all be accessed via a web browser.

Figure 1. The EU FP6 SEE-GRID Project Steering Committee

Figure 2. The new Blade Computer Cluster

The Lightweight Directory Access Protocol (LDAP) database for the Internet with applications was also implemented in 2004. The concept behind this development is to provide network information systems and use them to authenticate users on various CIR services. LDAP combines several systems that normally have to be maintained separately, and thus saves resources, increases efficiency and adds adaptability.

The Institute's new helpdesk is now running on Open source Ticket Request System (OTRS) with many features to manage customer telephone calls and e-mails.

TOP ACHIEVEMENTS

Development of new technology and equipment

Within the framework of CRO-GRID, the Institute has acquired a new HP Blade cluster and the acquisition of a Network Storage system is in progress[Fig 2].

Figure 3. Logo of the DCC software

Debian Cluster Components (DCC), an initial development version of a Linux Cluster Distribution was finalized as Open-Source, and is available on http://dcc.irb.hr/ [Fig 3].

Infrastructure support improvements

- A new Institute WEB site, based on Open-Source CMS, was presented March, 1 2004, after being programmed by CIR, (http://www.irb.hr/) [Fig 4].
- Testing of the Open Ticket Request System has been finished, and shall be introduced in 2005, as an integrated solution towards helpdesk and CIR services.
- Around 700 meters (length) was plotted through the CIR services [Fig 5].

Project initiatives

CIR submitted 2 new EU project proposals inside the ICT and LIFE programmes.

- FIRE-GRID project for forest fire early warning and prevention was submitted for the EU LIFE 3C programme, in cooperation with National Park Mljet.
- SATURN project (Seamless Access to a Trusted Ubiquitous Resources Network), lead by VTT Technical Research Centre of Finland was submitted for the EU IST FET programme.

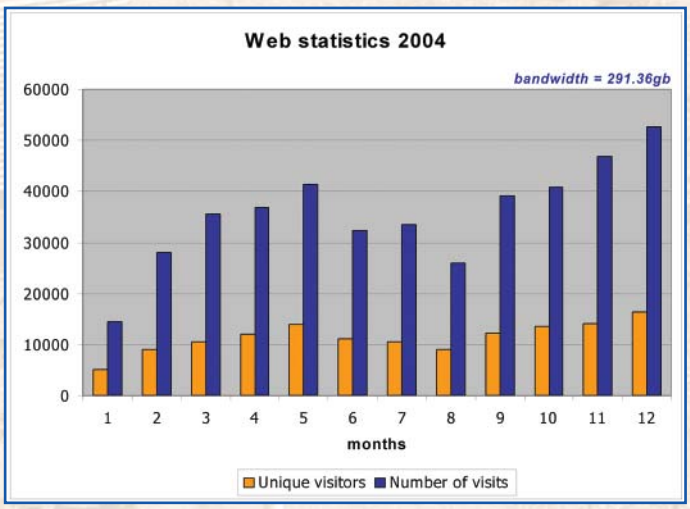

Figure 4. FTP, web and mail server statistics

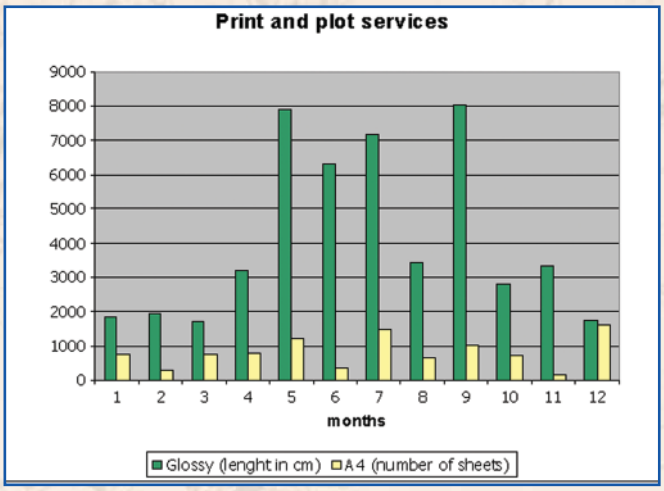

Figure 5. Summary of print and plot. Glossy paper plot length and A4 printed pages total

EDUCATIONAL ACTIVITIES

- The Center provides 4 undergraduate and 3 graduate courses at Faculty of Electrical Engineering and computing and Faculty of Graphical Arts at the University of Zagreb.
- Attendace at the 2nd International Summer School on Grid Computing 2004, Vico Equense, Italy 18 - 30 July 2004.
- For the RBI Open Days 2004, CIR produced a short film “Wise Choice”, intended for young future researchers to learn about the CIR activities, downloadable at http://www.irb.hr/en/cir/.

ORGANISATION OF CONFERENCES AND SPORTING EVENTS

CIR organized the annual Conference Hypermedia and Grid Systems as part of the International Convention MIPRO in Opatija (http://www.mipro.hr/ehgs.htm), and a traditional yearly gathering of the sailors from University and science at the University Sailing Regatta in Zadar.

SCOPE OF THE PROJECTS

Application scientific project

Detection of non-stationary sources and distributed information processing (2002-2005), Karolj Skala

Technological projects

1. Free space laser optical communications, HITRA, Karolj Skala
2. CRO-GRID Infrastructure, STRIP, Karolj Skala
3. CRO-GRID Applications, STRIP, Karolj Skala

Information technology projects

1. Parallel Random Forest algorithm, Goran Topić
2. Remote control and temperature measurement over WEB, Darko Kolarić

International projects

1. COST#276 Information and Knowledge Management for Integrated Media Communication, national coordinator, Karolj Skala
2. Grid enabled Infrastructure Development, SEE-GRID, EU FP6, con. no. 002356, Karolj Skala

Other Internal self-financing IT projects

1. Enhancements of the internal computer network
2. Server park development
3. Development of Cluster computing resources
4. LDAP data base implementation
5. Public LPD printing service establishment
6. Server monitoring system
7. Development DHCP and NAT services
8. New mail server installation

INVITED TALKS

Current State of the Most Interesting Applications for Croatian Grid, SoftCOM 2004, Venice, Italy, by Karolj Skala

PROTOTYPE, PATENT AND PRODUCT

- Optical Communication System in Diversity mode, Patent P20040692A, Državni zavod za intelektualno vlasništvo, 2004.
- Debian Cluster Components, Linux Cluster Distribution software package announced as an Open-Source product, and is available on http://dcc.irb.hr/.

COLLABORATION WITH OTHER INSTITUTIONS BASED ON CONTRACT

- Institute for Software Science of the University of Vienna, Austria
- Long-term contract for collaboration in the field of GRID technology, Ericsson - Nikola Tesla, Zagreb
- Memorandum of Joint ICT development, SRCE, Zagreb
- EU FP6 Consortium members SEE-GRID
- CRO-GRID Project Consortium member

SELECTED PUBLICATIONS

1. Skala K., Šojat Z., Towards a Grid Applicable Parallel Architecture Machine, Lecture Notes in Computer Science, Vol. 3038, Springer Verlag, 6-9 June 2004 p. 119 – 6.
2. Šojat Z., Skala K., Multiple Programme Single Data Stream Approach to Grid Programming, Biljanović P., Editor. Proceedings of the Hypermedia and Grid Systems 2004, Rijeka, p. 226–4.
3. Pavković, N., Vidić, V., Skala K., High Performance Cluster Distribution Design, New Frontiers CUC 2004, Zagreb, p 24.
4. Grubeša T., Jauk S., Ivančvić S., Simulation of Virtual 3D Auditory Spacs With HRTF, ELMAR

Center for Nuclear Magnetic Resonance

http://www.irb.hr/hr/nmr

Head of center: Dražen Vikić-Topić

OVERVIEW OF THE CENTER

The Center is the only academic NMR facility in Croatia. It provides support for scientists and researchers from the Ruđer Bošković Institute, from the Universities of Zagreb, Rijeka, Split and Osijek as well as governmental institutions and pharmaceutical industry. Research work at the NMR Center includes different topics in organic, inorganic and bioorganic chemistry as well as pharmaceutical chemistry. Theoretical calculations of molecular structures and NMR spectral parameters are carried out in order to support the experimental measurements. Investigations of natural compounds and photochemistry products are also in progress. In addition, the Center is involved in undergraduate and graduate studies of the Universities of Zagreb and Osijek. The Center's equipment includes Bruker Avance 300 and 600 MHz NMR spectrometers, purchased in 2002. The subsidiary of NMR Center, located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb, is using Varian's Gemini-300 MHz NMR spectrometer.

TOP ACHIEVEMENTS

Synthesis and photochemistry of styryl substituted compounds were performed as a model of an effect of annelation on intra- and/or intermolecular cycloaddition. These studies are part of a broader effort to track the photochemical pathways in biological systems. NMR and IR spectroscopic investigations of interactions of pharmaceutically active molecules were carried out as well. In this respect the antimicrobial peptides are of interest since, in some cases, small fragments can mimic and even supercede the activity of the whole molecule. Determination of the structure, bioactivity and sense-antisense interactions of short peptide fragments, with five to thirteen amino acids, were investigated.

ORGANIZATION OF INTERNATIONAL CONFERENCE AND COURSES

1. Summer School on Separation, Detection and Characterization: Principles and Applications in Pharmaceutical Chemistry and Life Sciences, Seggau, Austria, Sept 15-19, 2004
2. The 19th Dubrovnik International Course & Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Dubrovnik (IUC), July 21-26, 2004

PROJECTS

Domestic and international projects

1. Nuclear Magnetic Resonance and Calculations of Bioorganic Molecules, Dražen Vikić-Topić
2. Multi-Dimensional NMR Spectroscopy of Biomolecules, Dražen Vikić-Topić, Austrian-Croatian project

Technological projects

1. Plant Terpenes and Lignin as Natural Substrates for Biosynthesis of Anticancer and Industrial Intermediates, Dražen Vikić-Topić, EUREKA project.

Contracts with industry

1. Collaboration Contract with PLIVA d. d. Pharmaceutical Industry
2. Collaboration Contract with BELUPO d. d. Pharmaceutical Industry.

International collaborations

1. Institute of Chemistry, Johannes Kepler University, Linz, Austria
2. Faculty of Natural Sciences and Mathematics, Skopje, Republic od Macedonia
3. Department of Chemistry, Moscow State University, Moscow, Russia
4. National Institute of Chemistry, Hajdrihova 19, Ljubljana, Slovenia
5. Faculty of Science, Masaryk University, Brno, The Czech Republic
6. Mayo Clinic and Foundation, Rochester, MN, USA

TEACHING

1. Chemical toxicology: School of Health Studies, University of Zagreb, Dražen Vikić-Topić
2. Spectroscopic methods in structural analysis: Graduate Studies in Analytical Chemistry, Faculty of Science, University of Zagreb, Dražen Vikić-Topić
3. Application of NMR spectroscopy in determination of structure and dynamics of organic and bioorganic molecules: Graduate Studies in Organic Chemistry, Faculty of Science, University of Zagreb, Dražen Vikić-Topić
4. Modeling of protein structure and function - applications in biomedicine: Graduate Studies at School of Medicine, University of Zagreb, Dražen Vikić-Topić
5. Spectroscopic methods: Graduate Studies in Environmental protection, University of Osijek, Dražen Vikić-Topić

SELECTED PUBLICATIONS

1. Nemet I, Vikić-Topić D, Varga-Defterdarović L. Spectroscopic Studies on Methylglyoxal in Water and Dimethylsulfoxide. Bioorg. Chem. 2004: 32: 560.
2. Butković K, Basarić N, Lovreković K, Marinić Ž, Višnjevac A, Kojić-Prodić B, Šindler-Kulyk M. Photochemistry of β-(4-sydnonyl)-o-divinylbenzene: Competitive cis-trans Isomerisation and Photolysis. Tetrahedron Lett. 2004: 45: 9057.
3. Butković K, Marinić Ž, Šindler-Kulyk M. Complete 1H and 13C NMR spectral Assignment of cis- and trans-3-{2-[2-(4-methylphenyl)ethenyl]phenyl} Sydnones. Mag. Rec. Chem. 2004: 42: 1053.

Library

http://library.irb.hr

Head of Library: Jadranka Stojanovski

OVERVIEW OF LIBRARY ACTIVITIES

The RBI Library continues to make efforts to lead the way in the use of new technologies to develop resources and services which meet the needs of the RBI and the wider scientific community. The Library has followed strategic directions of providing easy access to high quality information in support of research and teaching, improving library services to facilitate intellectual life at the Institute, and being a leader in the use of information technologies.

The Library must provide the best possible access to the collections, under present-day conditions, for the purpose of research. At the same time, it must be ensured that the collections are preserved, secured and will be handed on to posterity. The RBI Library strives to build most relevant and comprehensive collections of scholarly literature available for research and further education for the country as a whole within the fields of physics, mathematics, electrical engineering, chemistry, biology, medicine, environmental and marine sciences.

The Library's book collection amounts to some 33500 volumes, 500 of which were newly acquired in 2004. E-books were reviewed for potential benefits to Library customers and some e-books were added to the collection in 2004. The journal acquisition model was turned toward e-journals completely, and additional printed versions were acquired only for small number of important titles for backup purposes. 9900 e-journal titles were funded by the Ministry of Science, Education and Sport via consortia agreements with major scientific publishers (Springer, Wiley, Kluwer, EBSCO, Elsevier), and 8400 e-journal titles were available free of charge and accessible through EJOL (Electronic Journal Online Library) and EZB (Elektronische Zeitschriften-bibliothek). The access to the relevant bibliographic and full-text databases was provided through the Centre for online databases (http://baze.irb.hr), maintained by the RBI Library for the academic and research community in Croatia. The RBI Library has a well-established inter-library loan service with Croatian and foreign libraries. In 2004 it fulfilled approximately 800 requests for documents made by members of the RBI, and over 700 requests from other libraries.

The Library is working systematically on an

Figure 1. 50th colloquium of the RBI Library

extension of the electronic services made available to the users. There were numerous other efforts to give our patrons better tools for accessing information and using the library, requiring less effort from them and allowing much of the basic library staff assistance to be given indirectly. This assistance included:

- Virtual reference collection,
- Timely updating of web pages,
- SEND interlibrary loan software,
- Subject portals
- Croatian libraries on the Web
- Croatian press online
- Education and training.

We continued national co-operation and partnership project Scientific Information System (SZI) which includes 120 libraries working on collections accessibility and library services improvement through five sub-projects (Biomedicine, Natural sciences, Engineering, Social sciences, Humanities). The main activities in 2004 were focused on co-operative subject portal ZIND using open source software and Content Management System (CMS) for small academic libraries.

We celebrated the 10th anniversary of the RBI Library web site and the 50th colloquium of the RBI Library simultaneously this year (Figure 1). Topics covered some historical survey, going back in 1994 when the RBI Library web site was launched as the first library web site in Croatia, as well as new and current work with CMS.

As a leader of two important projects, Croatian Scientific Information System (SZI) and Croatian Scientific Bibliography (CROSBI), in December we acquired two new servers Dell 2x Xeon 2.8 GHz as a gift from MSES. In the coming period we will move our existing information services to the new servers to improve performances and usage. Also in 2004 we purchased fourteen laptops primarily for educational purposes, giving RBI scientists the opportunity to increase the effectiveness of the learning processes in a variety of locations.

TOP ACHIEVEMENTS

Who's who in science in Croatia

With this project we intended to collect the data about Croatian scientists in a single location. The data are structured carefully to give good descriptions of each scientist's formal and continuing education, employments, teaching activities, projects, memberships, awards, scientific interests, intramural and extramural activities etc. The main goal is to improve communication between scientists as well as to promote Croatian scientists in the local community (Figure 2).

Figure 2. Who's who in science in Croatia

ZIND – Croatian Scientific Information Portal

Together with other libraries co-operating on the project Croatian Scientific Information System (SZI) we built a subject portal ZIND (http://zind.szi.hr) which should improve and make easier for the users the access to the numerous information resources available in the virtual web space.

Croatian Scientific Bibliography (CROSBI)

We continued to work on the project CROSBI (http://bib.irb.hr), which collects and publicly releases data about scientific papers resulting from research projects financed by the MSES. CROSBI has over 125000 records covering all scientific publications written by Croatian scientists.

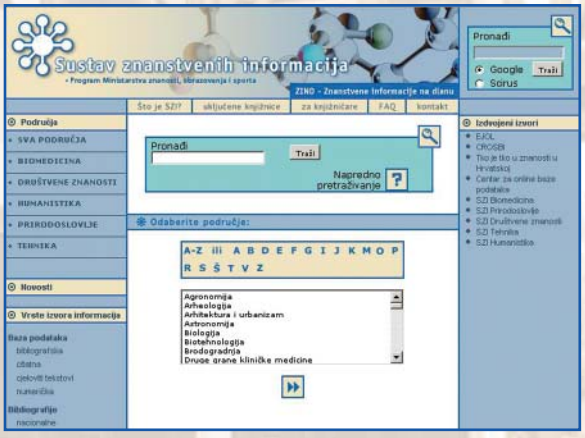

Figure 3. ZIND portal

AWARDS

Ivana Pažur: Eva Verona Award in 2004 – award for young librarians, for her outstanding dedication to work, innovative practice and promotion of library profession.

SELECTED LECTURES

1. Granić D, Mayer M, Vučina Ž. Distance learning and online databases retrieval example. Fifth Conference for Academic and Special Libraries; 2004 Nov. 5-6; Zagreb, Croatia.
2. Melinščak Zlodi I. Metadata: how to escape from and get closer to Google? Fifth Conference for Academic and Special Libraries; 2004 Nov. 5-6; Zagreb, Croatia.
3. Melinščak Zlodi I, Melinščak M. OAI@AKM. Archives Libraries Museums; 2004 Nov 24-26, Rovinj, Croatia.
4. Stojanovski J. Discovering Content Pattern of the Library Web Site. Libraries in the Digital Age LIDA; 2004 May 24-29; Dubrovnik and Mljet, Croatia.

CONFERENCE ORGANIZATION

The Fifth Conference for academic and special libraries: "Scientific information retrieval: what's in magician's hat?", Zagreb, 5-6 Nov 2004.

INFORMATION TECHNOLOGY PROJECTS

1. Croatian Scientific Bibliography CROSBI, Jadranka Stojanovski
2. Croatian Scientific Information System – Natural Sciences, Jadranka Stojanovski
3. Online Databases Center, Jadranka Stojanovski
4. Who's Who in Science in Croatia, Jadranka Stojanovski
5. EJOL Electronic Journals Online Library, Ivana Pažur and Sofija Konjević

SELECTED PUBLICATIONS

1. Konjević S. Croatian scholarly journals on the Internet. Vjesnik bibliotekara Hrvatske 2004: 46: 111

2. Mayer M. Chemistry Internet resources in Croatia. Kemija u industriji. 53 (2004) 3 126-128.
3. Melinščak Zlodi I, Melinščak M. OAI@AKM.. In: Katić T, editor. Proceedings of the Seventh Seminar Archives, Libraries, Museums; 2003 Nov. 26-28; Poreč, Croatia: Croatian Library Association; 2004, Zagreb. p. 192
4. Melinščak-Zlodi I. Where will publish chemicists of the future? Kemija u industriji 2004: 53:26
5. Pažur I. Authors of scientific papers and copyright. Vjesnik bibliotekara Hrvatske 2004: 47:95
6. Pažur I, Konjević S. EJOL - Electronic Journals Online Library. Kemija u industriji 2004: 53:226
7. Stojanovski J, Težak Đ. Self-citations and impact factors of Croatian journals. In: Proceedings of the Sixth CARNet User's Conference: New frontiers – New Technologies for New Needs: 2004 Sept. 27-29; Zagreb, Croatia: CARNet; 2004. (CD ROM edition).
8. Stojanovski J, Vodopijevec A. Library website usage statistics: users resources and citations. In: Lužar-Stiffler V, Hljuz Dobrić V, editors. ITI 2004 : poster abstracts of the 26th International conference on information technology interfaces; 2004 June 7-10; Cavtat, Croatia; SRCE University Computing Center University of Zagreb; 2004. p. 15
9. Stojanovski J. E-journals: publishers libraries and trends. Kemija u Industriji. 53 (2004) 10 460-461
10. Stojanovski J. Croatian chemical journals in ISI publications. Kemija u industriji. 53 (2004) 6 274-281

Notes

Notes

The Ruđer Bošković Institute (RBI) is the largest Croatian research centre in sciences and science applications. In the multi-disciplinary environment of the Institute more than 500 academic staff and graduate students work on problems in experimental and theoretical physics, chemistry and physics of materials, organic and physical chemistry, biochemistry, molecular biology and medicine, environmental and marine research, electronics, informatics and computer science. Within Croatia, the RBI is a national institution dedicated to research, higher education and provision of support to the academic community, to state and local governments and to technology-based industry. Within the European Union, the RBI forms a part of the European Research Area. Worldwide, the RBI collaborates with many research institutions and universities upholding the same values and vision.