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# Ruđer Bošković Institute

## Annual Report 2006





*Ruđer Bošković Institute*

## Annual Report 2006



Zagreb, 2007.

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Dear reader,

Welcome to the 2006 Annual report of the Ruđer Bošković Institute, which highlights the most important activities and achievements of Institute's Laboratories and Divisions in the past year. As the largest public Croatian research Institute in natural sciences, biomedicine, marine research and environmental sciences, which is mainly supported by the Croatian Ministry of Science, Education and Sports, our mission is mainly determined by the specific needs of the society in which we live. In particular, we aim to excel in three main directions: (i) production of high-quality fundamental research, (ii) involvement in higher education and (iii) contribution to the growth of the national economy through production of new technologies based on our own IP and expertise. Indeed, throughout 2006, the Institute was expected to preserve its leading role in performing excellent basic research. In addition, however, there were significant expectations to increase efforts towards commercialization of knowledge and production of intellectual property for the benefit of the national economy. At the same time, the existing and new knowledge and expertise acquired through basic research is expected to be efficiently transferred into the higher education sector through intensive collaboration with Croatian Universities. It is through the following pages, which highlight the results and activities of the Institute's Divisions and Laboratories, that we aim to demonstrate just how successfully we fulfilled our mission in 2006.

One of the most important events in 2006 was a call by the Ministry of Science, Education and Sports for new scientific projects. Along with the appraisal of the proposals for new projects, this required the evaluation of those projects contracted in 2002 and completed in 2006. The table found at the end of the Intro-

duction shows that, in terms of the completed projects, the RBI dominated in the top ten in physics, chemistry, biology, molecular medicine and oceanology. In terms of new applications, the RBI was also very successful with 122 projects granted contracts for the period 2007-2012. This success, taken together with the quality of scientific papers published in 2006, the number of invited lectures at international and domestic conferences and the fact that up to the end of 2006 a total of 16 EU FP6 projects were contracted, shows appreciable activity of RBI scientists in 2006.

Achieving a high rate of international collaboration is one of the RBI's ultimate goals. Within the forthcoming EU FP7 calls, we may expect further increase of international collaboration and stronger involvement of the RBI in the ERA.

In closing, I have the pleasant duty to thank the RBI scientific and administrative staff for their honest efforts and enthusiasm as well as their many excellent achievements throughout 2006. To you the readers of this 2006 Annual report I would like to express our sincere thanks for your interest and I would like to invite you to send us your critical opinions, suggestion for improvements and, by all means, proposals for future collaboration.

A handwritten signature in dark ink, appearing to read 'M. Žinić', written in a cursive style.

*Prof. Dr. Mladen Žinić*  
Director General

# Introduction

In 2006, the scientific and administrative staff of the RBI actively participated in the extension of the Institute's international collaboration and the intensification of various domestic activities, with efforts on both fronts aimed at increasing the RBI's contribution to the general development of the society. During 2006, the RBI was visited by more than 140 foreign scientists originating from the USA, Australia, and almost all European countries. As well as delivering well-received lectures, the visitors typically engaged in initiation or continuation of scientific collaboration. Within the framework of an agreement with the Embassy of France two distinguished French scientists, Prof. F. Fajula, from the Laboratoire de Matériaux Catalytiques et Catalyse en Chimie Organique, Institut Gerhardt, Ecole Nationale Supérieure de Chimie, Montpellier, France and Prof. P. Joliot, from the Institut de Biologie Physico-Chimique, Paris, France, visited the RBI and delivered their lectures in fully crowded lecture halls. The Institute was also very happy to host Dr. sc. A. R. Peaker, Director of the Centre for Electronic Materials, Devices and Nanostructures, School of Electrical and Electronic Engineering, University of Manchester, U.K., who is also a member of the RBI International Scientific Board and who delivered a most exciting lecture entitled "Semiconductor Materials Research at the University of Manchester" and discussed related scientific issues with RBI physicists.

The RBI also hosted several international delegations, among them the Working group on Assistance to Central & Eastern Countries of the Federation of European Biochemical Societies, headed by Prof. Guy Dirheimer (France) and consisting of members from the Netherlands, Poland, Israel, Ukraine, the

United Kingdom, Romania and Austria. The Institute was also visited by the president of the Science Foundation of Ireland, Dr. William C. Harris, M. D. Lindeman, Senior Program Director for Development and External Relations of US Civilian Research & Development Foundation and a delegation of the Styrian Joanneum Research headed by the Scientific director Prof. Bernhard Pelzl, and the Administrative director Edmund Müller. On that occasion, sufficiently many points of common interest between Joanneum Research and RBI were identified so as to merit the initiation of a close collaboration, especially in the fields of nanotechnology, ecology, medicine diagnostics and sensor development. In 2006, the Institute also had the honour to host the new Ambassadors of Japan and the Republic of India, their excellences Tetsuhise Shirakawa and Rajiva Misra. The bilateral collaborations between the RBI and scientists of Japan and India were discussed on those occasions.

The participation of RBI scientists in European scientific networks remained one of the Institute's top priorities in 2006. RBI continued active collaborations in different COST actions and succeeded to contract an additional 6 FP6 projects reaching the total number of 16 FP6 projects contracted up to the end of 2006. It is also of prime importance that in 2006, the RBI became a member of the EMBL association. RBI scientists also took active role in Management Committees of COST actions, Prof. K. Pavelić, head of the RBI's Division of Molecular Medicine was re-elected vice president of EMBO and Prof. T. Legović, head of the Division of Marine and Environmental Research was appointed Secretary General of the International Society for Ecological Modelling.



Further fostering activities toward exploration of different ways of commercialization of knowledge RBI undertook several important steps in 2006. As the participant in the Science and Technology Project contracted by Croatia and the World Bank in March 2006, the RBI established Rudjer Innovations Ltd. as the Agency for protection and commercialization of RBI-produced IP and expertise. In parallel, 28 RBI employees participated in CARDS program Intellectual Property Rights - Infrastructure for R&D Community in Croatia. To define and protect the rights of inventors work on RBI internal IP regulations was started. Although still in the initial phase, the RBI activities toward generation of IP increased in 2006 resulting in a total of 9 inventions currently in different phases of realization. One of the major achievements in 2006 was the development and testing of an advanced apparatus for photodynamic diagnosis and therapy (PDT and PDD) of skin malignant diseases under the brand name - MediLED-7<sup>®</sup>. The device is going to be completed with new software in 2007. Construction of QRBG121 – Quantum random number generator, a fast non-deterministic random number generator with bit rate of 12Mb/s presents one of the RBI's strong candidates for commercialisation. It is also encouraging that in 2006 two new spin-offs were established by RBI scientists: Chirallica Ltd. producing HPLC columns with chiral stationary phases and performing separation of chiral pharmaceuticals and Communication Technologies Ltd. for the development of ICT products.

In 2006 the RBI signed a contract on cooperation with one of the largest Croatian companies, the Concern Agrokor, initiating collaboration in food quality control and joint development of new products; in this year already two projects were realised. Previous successful collaboration between the RBI and glass Producer Company Lipik Glass was formalized and a new project started in

2006. Also short term project collaboration with pharmaceutical company PLIVA continued successfully in 2006.

The RBI's expertise in ecology and environmental sciences was offered to the City of Zagreb, which resulted in the signing of an agreement on future collaboration. The cooperation with the Croatian Conservation Institute was formalized in the form of collaboration contract. Under the IAEA technical cooperation project, analytical capabilities of both Institutes have been upgraded. A new mobile XRF system has been provided for CCI, while the construction of new in-air PIXE beam line and upgrade of ion microprobe has been completed at RBI. Recent joint projects include characterization of the Apoxiomenos statue found several years ago in the Northern Adriatic and analysis of pigments in paintings of Master HGG. Both projects resulted in exhibitions presented to public in 2006. It is noteworthy to mention that RBI contributed to exhibitions "Science in images – look at hidden reality" held in Split and "Art of Science and Power of Knowledge" organized in Zagreb. To promote research and inventive endeavour in Croatia especially in ICT, the Institute founded the E-novation Award together with the VIDI Magazine; the first Award was granted in December 2006. In accord with the strategy to contribute to further development of research and higher education in all Croatian regions, a Letter of Intent predicting future collaboration with the Region of Istria and its newly established University in Pula was signed and supported by the Croatian Ministry of Science Education and Sports. And last but not least, the RBI actively participated in the organization of events dedicated to 100<sup>th</sup> anniversary of the birth of the world renowned organic chemist, former ETH professor and Nobel Prize winner, the late Professor Vlado Prelog our countryman who strongly contributed to the development of chemistry research and the pharmaceutical industry in Croatia.



## 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 573, including 361 researchers, 212 Ph.D. students, 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, with an important role played by the International Scientific Board. Their organizational integration with the remainder of the Institute is displayed below.

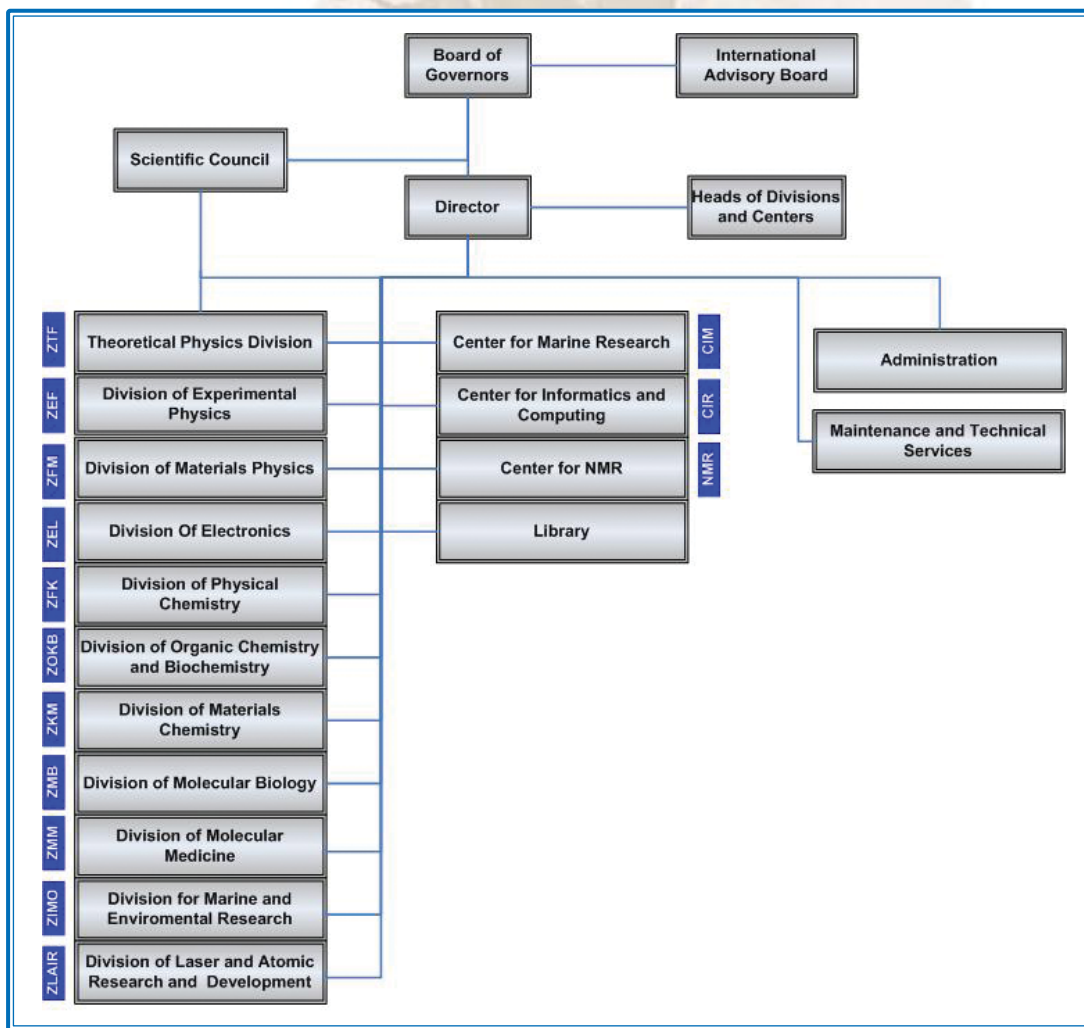


Figure 1. The organizational structure of the RBI

## ORGANIZATION OF THE INSTITUTE

Director: Mladen Žinić

Head of the Scientific Council: Maja Osmak

Chairman of the Board of Governors: Janko Herak (until November); Slavko Krajcar

### International Scientific Board.

- Jean-Marie Lehn, Laboratoire de Chimie Supramoléculaire, ISIS/ULP, France
- Harold Kroto, University of Sussex, UK
- Egon Matijević, Clarkson University, NY, USA
- Helmut Schwarz, Technische Universität Berlin, Germany
- Fritz Vögtle, Universität Bonn, Germany
- Julius Erich Wess, MPI für Physik, Werner-Heisenberg-Institut, Germany
- Robert Blinc, Jozef Stefan Institute, Ljubljana, Slovenia
- Jonathan R. Ellis, CERN, Switzerland
- A.R. Peaker, University of Manchester, UK
- Bogdan Povh, MPI für Kernphysik, Heidelberg, Germany
- Fernando Azorin, Institute of Molecular Biology of Barcelona, Spain
- Bernd Kaina, Institut für Toxikologie, Mainz, Germany
- Werner E.G. Müller, Johannes Gutenberg Universität, Mainz, Germany
- Miroslav Radman, Université René Descartes-Paris V, France
- Jürgen Soll, Ludwig-Maximilians-Universität München, Germany
- Vito Turk, Jozef Stefan Institute, Ljubljana, Slovenia
- Joseph Schlessinger, Yale University School of Medicine, CT, USA
- Hans Joachim Seitz, Universität Hamburg, Germany
- Davor Solter, MPI für Immunbiologie, Freiburg, Germany
- Peter J. Stambrook, University of Cincinnati Medical Center, OH, USA

- Rudolf Zechner, Institute for Molecular Biosciences, Graz, Austria
- Farooq Azam, University of California, San Diego CA, USA
- Walter Giger, Swiss Federal Institute for Aquatic Sciences and Technology, Dübendorf/Zürich, Switzerland
- Thomas C. Malone, OceanUS Office for Integrated and Sustained Ocean Observations, Arlington, VA, USA
- Werner E.G. Müller, Johannes Gutenberg Universität, Mainz, Germany
- Nadia Pinardi, University of Bologna, Ravenna, Italy

## ACTIVITIES

### Fundamental research

The total number of research articles published in 2006 was 489. Among these, 355 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 to note that 23% of all Croatian articles in Current Contents journals originated from the RBI. The majority of the scientific results produced in 2006 were published in high ranking international Journals. Besides, the RBI scientists were authors of four scientific books and 22 book chapters.

Several important discoveries contributed by RBI scientists were accomplished in 2006. The scientists from Theoretical Physics and Experimental Physics Divisions published 4 papers in the most prestigious scientific journal for physics that of Physical Review Letters. They published the first complete leading-twist next-to-leading-order PQCD predictions for the two-photon exclusive channels  $\gamma\gamma \rightarrow M^+ M^-$  ( $M = \pi K$ ) at large momentum transfer and in another work a realistic calculation of the ultra fast electron response at Cu(111) surface has been car-

ried out. Using the multi-channel, multi-resonance coupled-channel partial wave analysis was developed entirely in the Division of Experimental Physics. Another interesting result developed from the analysis of data from the measurement of the  ${}^6\text{He}+{}^6\text{Li}$  reactions (see the following reports of Theoretical and Experimental Physics Divisions). One of the most interesting discoveries was published in Nature (2006: 443: 569; see the report of the Division of Molecular Biology) revealing how bacterium *Deinococcus radiodurans*, one of the most radiation resistant organisms known, restores its genome shattered by radiation. The results present the outcome of a fruitful collaboration between RBI and French scientists at the Faculté de Médecine Necker-Université Paris 5 led by the Croat and member of the RBI International Scientific Board, Prof. M. Radman. More details concerning these few excellent results, along with selected others, are presented in the following reports of the individual Divisions and Centres.

## Projects

In 2006 the RBI completed 122 projects in basic research, which were funded by the Ministry of Science, Education and Sport (MZOS) during the 2002-2006 period. According to the evaluation of MZOS at the end of project period, many of the RBI projects were ranked in the top 10 within their respective fields. In March, a new MZOS call for proposal was opened for the period 2007-2012. For the first time, the international evaluation of proposals was implemented. RBI scientists successfully applied for new projects and 122 were accepted for MZOS financial support. In comparison to the 2002-2006 period, the total research funding contracted for 2007-2012 is somewhat higher. In addition to the fundamental projects, the Institute is involved in 74 international projects (50 bilateral, 16 FP6, 7 IAEA, 1 UNESCO), as well as 37 applied and technological projects.

## Education

In 2006, 177 scientists from the Institute contributed 99 undergraduate courses and 190 graduate courses to the program of higher education in Croatia. Their respective distributions amongst the five universities at which they were delivered, as well as by the divisions and centers that contributed, are shown in Figures 2, 3, 4 and 5. In addition to the coursework, 47 B.Sc., 29 M.Sc. and Ph.D. theses were completed under the supervision of the RBI academic staff in 2006.

In 2006, joint PhD studies of the Ruđer Bošković Institute, the University of Osijek and the University of Dubrovnik began in the field of Molecular Biosciences ([www.unidu.hr/molekularna/index.html](http://www.unidu.hr/molekularna/index.html)). More than thirty students from all regions of the Croatia signed for studies in 2006, while the first

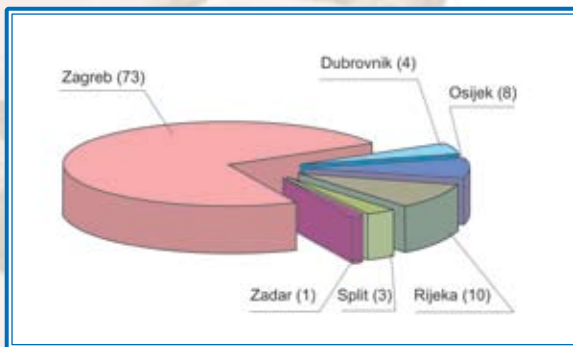


Figure 2. Distribution of the RBI held undergraduate courses (99) at domicile Universities.

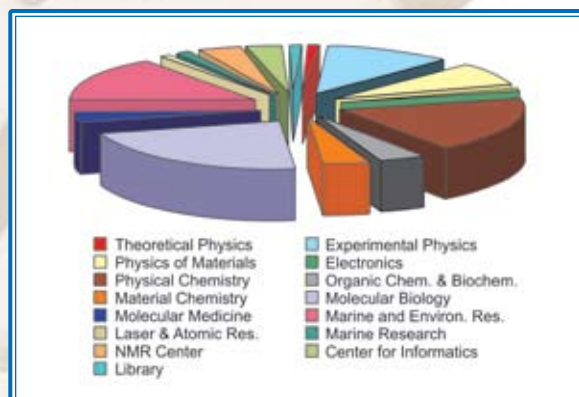


Figure 3. Distribution of the RBI-held undergraduate courses (99) by RBI Divisions and Centres.



workshop denoted “Mentorship Fair” organised to provide mentors for all students was held at the Institute in September 2006. In parallel the agreement on joint PhD studies was also signed with Universities of Split, Zadar and Dubrovnik. The PhD study on “Biology of Neoplasm” began to sign students in autumn 2006 expecting to start in 2007. The interdisciplinary postgraduate study on the Oceanology in collaboration with the Faculty of Natural Sciences University of Zagreb, Institute for Marine and Coastal Research of the Dubrovnik University and Institute of Oceanography and Fisheries in Split were founded in 2006.

In 2006, the Institute continued successful graduate studies in Project Management

organised as joint studies with College of Business and Management “Baltazar Adam Krčelić”. The progress of this program in the initial academic year (2005/06) led to a 50% increase in the number of students that signed-on for the second generation of Project Management studies. Of particular relevance was organisation of the “INFO day about the applicability of European projects for R&D in Croatia” in September. Besides our lecturers and experts from the Ministry of Science, Education and Sports, as well as Ministry of Foreign Affairs and European Integrations, special lecture about the development of European Research Area and Croatian opportunities was given by Dr. Raoul Kneucker, member of the European Commission Working Group for the Lisbon Strategy and supervisor of the Project Management studies.

### Organization of international conferences

As in previous years, the RBI continued to support the organization of 18 international and domestic conferences. Among the most noteworthy of these were the 150<sup>th</sup> anniversary of the birth of great inventor Nikola Tesla and the 100<sup>th</sup> anniversary of the birth of the Nobel-Prize winner for chemistry, Vladimir Prelog. The 9<sup>th</sup> International Summer School on Biophysics: Supramolecular structure and function, held in Rovinj, from 16-28 September 2006, was successfully organized, as many times before, by Professor G. Pifat-Mrzljak. Along with the importance of permanent education of young scientists from all around the world in the field of biosciences via interdisciplinary approaches offered by international experts, the School is recognized and accepted as a part of curriculum of distinguished European universities (e.g. University of Leeds, UK, University of Osnabrück, Germany, University of Lisbon, Portugal, University of Maribor, Slovenia, Universities of Zagreb and Rijeka, Croatia).

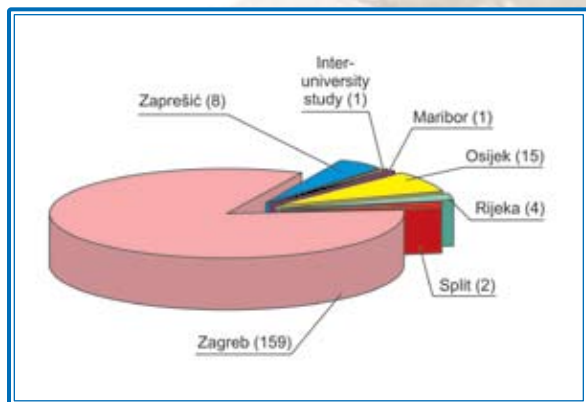


Figure 4. Distribution of the RBI held graduate courses (190) at domicile Universities.

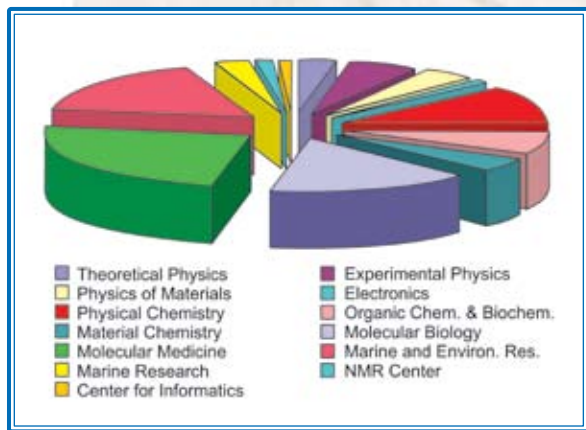


Figure 5. Distribution of the RBI held graduate courses (190) by Divisions and Centres.

The 21<sup>st</sup> Dubrovnik International Course & Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences took place in Dubrovnik (IUC), July 19-24, 2006 as well as the 5<sup>th</sup> International DU NMR Course and Conference in Mali Ston in November 02-05, 2006. Both conferences are already traditional with many participants from Croatia and abroad.

The biannual international conference "From solid state to Biophysics III" which organization is co-supported by Ruđer Bošković Institute, École Polytechnique Fédérale de Lausanne, Switzerland, Faculty of Science, Zagreb, Institute of Physics, Zagreb, and the University of Dubrovnik, took place on June 21-July 1 in Cavtat near Dubrovnik. The 50<sup>th</sup> IUVESTA workshop "Toward Novel Nanostructure-based Devices: Nanostructured materials fabrication, characterization and assembly for novel devices", was co-organized by B. Pivac and N. Radić and held in Dubrovnik, 22-27 October 2006. Also, the School on Particle Physics, Gravity and Cosmology, was held in Dubrovnik, Croatia, August 21 – September 2, 2006. The School is organized by Physics Department, Faculty of Science, University of Zagreb, and International School for Advanced Studies (SISSA), Trieste, Italy in collaboration with the Theoretical Physics Division of the RBI.

## NEW EQUIPMENT

The Molecular Physics Laboratory of the Division of Physics of Materials became richer with the acquisition of a new Raman spectrometer, T64000 from HORIBA-Jobin Yvon, which was installed in December of 2006. The attainment of this valuable equipment was financially supported by the Ministry of Science Education and Sports. With its high, research oriented flexibility; it will promote materials science at the Ruđer Bošković

Institute and in Croatia as a whole. Detection of scattered light crucial for Raman spectroscopy is now enhanced by alternative use of two CCD detectors, covering spectral the region from UV to NIR. Thus, previously inaccessible samples such as opaque or sensitive materials can be studied using smaller laser power at the focus, while the recording time is greatly reduced for others. The system includes microscope with automated XY stage, onto which a variable temperature cell (90 K – 600 K) can be mounted. In this way one can record spectra for a chosen sample surface and analyze the surface composition and temperature changes.

Also the infrastructure of the Division of organic chemistry and biochemistry was greatly improved by acquisition of a new CD spectrophotometer Jasco J 815, which was financially supported by the Ministry of Science, Education and Sports. This CD spectrophotometer represents the first such piece of equipment available for use by the Croatian academic community and it will significantly improve the quality of research of optically active compounds.

## PUBLICATION RESULTS OF RBI FUNDAMENTAL RESEARCH PROJECTS

The following list was prepared according to the final status of the 2002-2006 project term using data from the National Bibliography database (web address: <http://bib.irb.hr/statistika?sto=p&pperiod=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 2002-2006, and the number of articles is the total number of scientific papers published in this particular project in 2006. 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 CROSB Bibliography on February 15th 2007	Number of CC Articles Published in 2006
BIOLOGY - 60	Structure and function Of plastids and cytoskeleton	Nikola Ljubešić	4.	6
	Study of genes and genomes of evolutionary preserved and economically important organisms	Vera Gamulin	5.	5
	Dynamics and genetics of bioactive molecules	Volker Magnus	7.	1
	Regulation of recombinant and recombinational repair	Mirjana Petranović	9.	5
	Cellular responses to physical, chemical and biological noxis	Maja Osmak	10.	4
BIOMEDICINE - Neuroscience - 58	Neuropharmacology of serotonin system	Dorotea Mück-Šeler	1.	7
	Molecular pathophysiology of serotonergic transmission	Branimir Jernej	8.	2
	Oxidative/antioxidative status after treatment with opioids/opiates	Tatjana Marotti	10.	4
BIOMEDICINE - Oncology - 73	Influence of gene/protein transduction on signalling Pathways of transformed cells	Krešimir Pavelić	1.	10
	Gene therapy of tumors by correction of tumor-Suppressor gens	Jasminka Pavelić	2.	14
	Oxidative stress and malignant disease	Neven Žarković	3.	8
	Regulation of ectopeptidases and opioid receptors expression	Jelka Gabrilovac	7.	6
CHEMISTRY - 75	Proton affinity and proton transfer reaction in chemistry	Zvonimir Maksić	1.	10
	Reactivity and reaction mechanisms	Dunja Srzić	2.	12
	Supramolecular organization in gels, molecular recognition and catalysis	Mladen Žinić	4.	14
	Structure and dynamics of (bio)molecules	Biserka Kojić-Prodić	5.	10
	Synthesis and microstructure of metal oxides and oxide glasses	Svetozar Musić	6.	9
	Nuclear Magnetic Resonance and calculations of bioorganic molecules	Dejan Plavšić	7.	11



	Development and application of models in chemistry and bioinformatics	Nenad Trinajstić	8.	5
	Reactive intermediates in Ground and excited states	Mirjana Maksić	9.	6
	Electron spin resonance in systems with paramagnetic particles	Boris Rakvin	10.	6
<b>GEOLOGY &amp; OCEANOLOGY - 56</b>	Mechanism of long-term changes of the Adriatic-sea ecosystem	Danilo Degobbi	2.	7
	Geochemistry of recent and ancient sedimentation systems of the Adriatic platform	Goran Kniewald	3.	8
	Physics and biogeo-chemistry of trace metals in aquatic systems	Ivanka Pižeta	4.	10
	Programmed biosynthesis and genotoxic risk	Renato Batel	5.	1
	Nature and reactivity of organic compounds in seawater and environment	Božena Čosović	6.	5
	Research of the ebb and long-periodical dynamics of northern Adriatic	Milivoj Kuzmić	8.	3
<b>PHYSICS - 88</b>	Fundamental interactions in physics of elementary particles and in cosmology	Branko Guberina	2.	13
	Influence of defects and nanostructures on characteristics of semiconductors	Branko Pivac	3.	12
	Heavy ion physics	Zoran Basrak	4.	9
	Light atomic nuclei: clusters, nuclear molecules, reactions...	Đuro Miljanić	5.	9
	Physics and applications of nanostructures	Krešimir Furić	7.	9
	Quantum field theory, noncommutative spaces, and symmetries	Stjepan Meljanac	8.	2
	High energy experimental physics	Krešo Kadija	9.	7
<b>INFORMATION &amp; COMPUTER TECHNOLOGY - 16</b>	Automated knowledge discovery and reasoning	Nikola Bogunović	1.	0
<b>TRANSPLANTATION OF GENES AND TISSUES - 26</b>	Assessing functions of the heat repeat in Huntingtin protein	Oliver Vugrek	10.	3

TABLE 1: Publication results of RBI fundamental research projects ranked among the top 10 Croatian projects in their respective field of science.

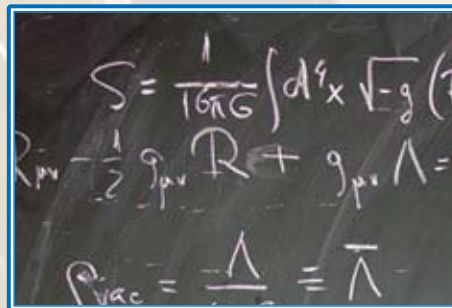


## DIVISIONAL ORGANIZATION

Head: Branko Guberina

The 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



## TOP ACHIEVEMENTS

**The first complete leading-twist next-to-leading-order PQCD for  $\gamma\gamma \rightarrow M^+ M^-$**

Exclusive processes at large momentum transfer provide a particularly suitable testing ground for perturbative QCD (PQCD). The leading-order (LO) PQCD predictions have been obtained for many exclusive processes, but owing to their sensitivity to the choice of the renormalization scale and scheme, they do not have much predictive power. To stabilize the LO results, and to achieve a complete confrontation between theoretical predictions and experimental data, it is crucial to take into account higher-order contributions.

We have obtained the first complete leading-twist next-to-leading-order PQCD predictions for the two-photon exclusive channels  $\gamma\gamma \rightarrow M^+ M^-$  ( $M = \pi K$ ) at large momentum transfer. The asymptotic distribution amplitude is utilized as a candidate form for the nonperturbative dynamical input. Comparison of the obtained results with the existing experimental data does not provide sufficiently clear evidence for the applicability of the hard-scattering approach at currently accessible energies (Duplanić G and Nižić B, Phys Rev Lett 2006: 97: 142003).

## 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. In addition, there is substantial research activity in condensed matter physics. A special activity in the Division is the nature of medical modelling in life science and the application of nonlinear statistical methods in biomedicine. In 2006, 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.



## Phantom gravastars

New gravitational vacuum star solutions have been constructed with a Born-Infeld phantom replacing the de Sitter interior. The model allows for a wide range of masses and radii required by phenomenology, and can be motivated from low energy string theory. (Bilić N et al., JCAP 2006: 02: 013).

## Cosmology within a modified gravity

A modified gravity model with the scaling Newton constant  $G_N$  and the constant vacuum energy (cosmological constant), which acts as a dynamical dark energy model, is applied in cosmology. It has been shown that, using the observational bounds on  $G_N$ , the effective field theory infrared cut-off becomes strongly restricted, approaching closer the future event horizon rather than the Hubble distance. For nonzero curvature, the model accommodates a transition across the phantom line for red-shifts smaller than  $z=2$ . (Guberina B et al., Phys Lett B 2006: 636: 80).

## Relativistic acoustic horizons

Transonic accretion onto astrophysical objects is a unique example of analogue black hole realized in nature. In the framework of relativistic acoustic geometry, axially symmetric accretion of a rotating astrophysical black hole has been studied assuming isentropic flow. Retarded and advanced null curves clearly demonstrate the presence of the acoustic black hole at regular sonic points and of the white hole at the shock. The analogue surface gravity and the Hawking temperature have been calculated for the inner and the outer acoustic horizons. (Abraham H et al., Class Quantum Grav 2006: 23: 2371).

## Matrix oscillator and Laughlin Hall states

A quantum matrix oscillator has been proposed as a model that provides the construction of the quantum Hall states in a direct way. A connection of this model to the regularized Chern-Simons matrix model is established and it has been shown that the quantum matrix oscillator describes the quantum mechanics of electrons in the lowest Landau level with the ground state described by the Laughlin-type wave function (Meljanac S and Samsarov D, Phys Lett A 2006: 351: 246).

## Giant gravitons and duality

The dynamics of giant gravitons has been studied using the matrix model in the collective-field formulation. We have analyzed two types of gravitons represented by different types of Young tableaux. These two types of giant gravitons are dual to each other. Using the duality properties of the BPS equation, we have formulated conformal fields and found the n-soliton solutions from the Riccati equation. The singular limit of some of these solutions is examined and a realization of the open/closed string duality is proposed (Andrić I et al., JHEP 2006: 0612: 006).

## New realizations of Lie algebra kappa-deformed Euclidean space

A kappa-deformed Euclidean space with undeformed rotation algebra  $SO_a(n)$  and with commuting vector-like derivatives has been analyzed. Infinitely many realizations in terms of commuting coordinates have been constructed and a corresponding star product has been found for each of them (Meljanac S and Stojić M, Eur Phys J C 2006: 47: 531).

## Electronic dynamics on the femto-second scale

The study of the ultrafast response of electrons in solids is one of the new frontiers of condensed matter research, prompted by the development of ultrashort laser pulses and novel detection techniques. Methods such as pump-probe two-photon photoemission (2PPE) have enabled experimental determination of electron dynamics on the time scales shorter than the onset of the usual relaxation regime. Based on a many-body description of the nonadiabatic dynamics of quasiparticles in surface bands, a realistic calculation of the ultrafast electron response at Cu(111) surface has been carried out by Predrag Lazić in collaboration with scientists from the Institute of Physics in Zagreb and from the Donostia International Physics Centre in San Sebastian, Spain (Lazić P et al., Phys Rev Lett 2006: 97: 086801).

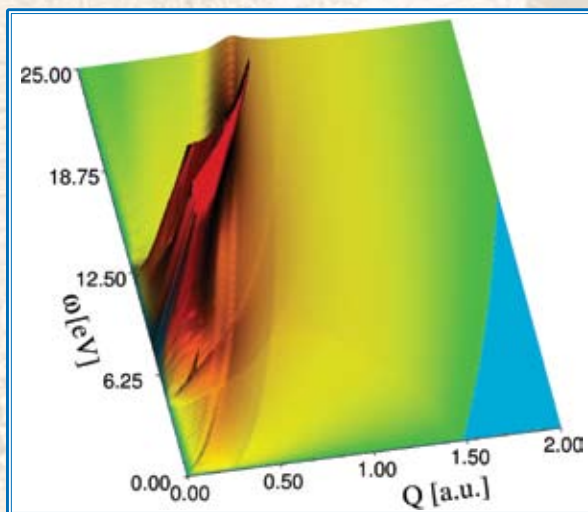


Figure 1: Response of the electrons on Cu(111) surface which governs the dynamics of an excited image state. The prominent features at small  $Q$  are due to the surface monopole and dipole plasmon excitations.

## (Multi)fractality of physiological time-series

The application of the fractal concept in analyzing heartbeat (RR interval) fluctuations measured under controlled physical activity for subjects with stable angina pectoris (SAP) is attempted. Results that illustrate the separation ability of the nonlinear methods, such as the Hurst  $R/S$  method, the detrended fluctuation analysis, DFA, and the method of  $G$ -moments, in distinguishing healthy from SAP subjects in scaling parameter space have been presented (Knežević A and Martinis M, Int Journal of Bifurcation and Chaos, 2006: 16: 2103).

## 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
5. Dark matter and the formation of structures in the Universe, Davor Palle

### Research, developmental and international projects

1. Anđelka Andraši: Fundamental questions of non-abelian quantum gauge theories and cosmology, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Eötvös Loránd University, Budapest, Hungary.



2. Neven Bilić: Scientific Joint Project: Investigations on the Nature of Dark Matter and Dark Energy (DMDE) between the Particle Physics and Cosmology Group, Theoretical Physics Division of the Ruđer Bošković Institute and the Astrophysics Sector of the International School for Advanced Studies (SISSA), Trieste, Italy.
3. Branko Guberina: collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and the Jozef Štefan Institute, Ljubljana, Slovenia, Hard-hadron physics in the standard model and beyond.
4. Blaženka Melić: International Research Project: "QCD sum rules for exclusive decays of heavy hadrons" promoted by the Alexander von Humboldt Foundation. Principal investigators: Dr. Sc. B. Melić and Prof. Dr. Th. Mannel (Uni. Siegen).
5. Stjepan Meljanac: Aspects of Calogero models, noncommutative geometry and quantum physics, Indo-Croatian Programme of Cooperation in Science and Technology for collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Saha Institute of Nuclear Physics, Calcutta, and Institute of Mathematical Sciences, Chennai, India.
6. 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".
7. Zoran Škoda: Nonabelian Cohomology and Applications in Geometry, Algebra and Physics, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Universität Hamburg, LMU München and Universität Göttingen, Germany.
3. J. Trampetić: Possible signals for space-time noncommutativity in particle physics, Symposium 2006 für Peter Minkowskis "Emeritierung", Spontaneous topics in theoretical physics, Bern, Switzerland, May 5, 2006.
4. N. Bilić: Chaplygin-gas cosmology: unification of dark matter and dark energy, 2nd International Conference on Quantum Theories and Renormalization Group in Gravity and Cosmology, Barcelona, Spain, July 11-15, 2006.
5. B. Guberina: Renormalization group running cosmologies - from a scale setting to holographic dark energy, invited plenary talk at the 2nd International Conference on Quantum Theories and Renormalization Group in Gravity and Cosmology, Barcelona, Spain, July 11-15, 2006.
6. H. Štefančić: What is in the black box of dark energy: variable cosmological parameters or multiple (interacting) components?, 2nd International Conference on Quantum Theories and Renormalization Group in Gravity and Cosmology, Barcelona, Spain, July 11-15, 2006.
7. N. Bilić: Black-hole phenomenology, School on Particle Physics, Gravity and Cosmology, Dubrovnik, Croatia, August 21 – September 2, 2006.
8. Z. Škoda: Realizations of noncommutative spaces, IV Summer School in Modern Mathematical Physics, Zemun, Serbia, September 3-14, 2006.
9. J. Trampetić: Signals for space-time noncommutativity in particle physics, IV Summer School in Modern Mathematical Physics, Zemun, Serbia, September 3-14, 2006.
10. B. Melić: Theoretical status of B meson physics, The 2006 LHC Days in Split, Split, Croatia, October 2-7, 2006.
11. J. Trampetić: Improved Z  $\rightarrow$  gamma gamma decay in the renormalizable gauge sector of the noncommutative standard model, The 2006 LHC Days in Split, Split, Croatia, October 2-7, 2006.
12. B. Melić: Introduction to  $\phi^2$  from charmless decays, 4th International Workshop on the CKM Unitarity Triangle, Nagoya, Japan, December 12-16, 2006.
13. B. Melić: QCD Light-Cone Sum Rules for Charmless Decays - most recent improvements, 4th International Workshop on the CKM Unitarity Triangle, Nagoya, Japan, December 12-16, 2006.

## SELECTED INVITED LECTURES

1. Z. Škoda: Lie algebra representations via deformations within Weyl algebra, Workshop "Noncommutative Algebras", Muenster, Germany, February 2-6, 2006.
2. J. Trampetić: Signals for Noncommutativity in Particle Physics, Bayrischzell Workshop 2006 "Noncommutativity and Physics", Bayrischzell, Germany, April 21-25, 2006.



## SELECTED ORGANIZED CONFERENCES

1. School on Particle Physics, Gravity and Cosmology, Dubrovnik, Croatia, August 21 – September 2, 2006. The School is organized by: Physics Department, Faculty of Science, University of Zagreb, Croatia and International School for Advanced Studies (SISSA), Trieste, Italy in collaboration with the Theoretical Physics Division of Ruđer Bošković Institute, Zagreb, Croatia.

## SELECTED PUBLICATIONS

1. Abraham H, Bilić N, Das T K: Acoustic horizons in axially symmetric relativistic accretion. *Class Quantum Grav* 2006: 23: 2371.
2. Andrić I, Jonke L, Jurman D: Solitons and giants in matrix models. *J High Energy Phys* 2006: 0612: 006.
3. Bilić N, Tupper G B, Viollier R D: Born-Infeld phantom gravastars. *JCAP* 2006: 02: 013.
4. Duplančić G, Nižić B: NLO perturbative QCD predictions for  $\gamma\gamma \rightarrow M^+ M^-$  ( $M=\pi K$ ). *Phys Rev Lett* 2006: 97: 142003.
5. Grigoriev A, Skoldberg J, Wendin G, Crljen Ž: Critical roles of metal-molecule contacts in electron transport through molecular-wire junctions. *Phys Rev B* 2006: 74: 045401.
6. Guberina B, Horvat R, Nikolić H: Dynamical dark energy with a constant vacuum energy density. *Phys Letters B* 2006: 636: 80.
7. Knežević, A, Martinis, M: (Multi)fractality of physiological time-series. *Journal of Bifurcation and Chaos* 2006: 16: 2103.
8. Lazić P, Silkin V M, Chulkov E V, Echeniue P M, Gumhalter B: Extreme ultrafast dynamics of quasiparticles excited in surface electronic bands. *Phys Rev Lett* 2006: 97: 086801.
9. Meljanac S, Samsarov A: Matrix oscillator and Laughlin Hall states. *Phys Letters A* 2006: 351: 246.
10. Meljanac S, Stojić M: New realizations of Lie algebra kappa-deformed Euclidean space. *Eur Phys J C* 2006: 47: 531.





## DIVISIONAL ORGANIZATION

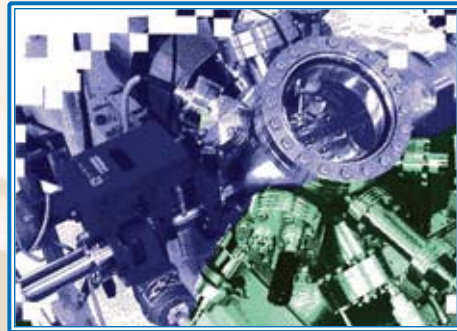
Head: Alfred Švarc

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

The mission of the Division of Experimental Physics is twofold: high quality basic research in experimental nuclear and particle physics, and application of acquired experience in nuclear techniques to other areas of science and economy. Both activities are successfully carried out through international collaborations and in Croatia. In basic



research a number of breakthroughs were achieved in 2006, with the accompanying results being published in high quality scientific journals. In applications, present activities were strengthened, a number of important projects were initiated, and several financially very favorable international research contracts were realized.

## TOP ACHIEVEMENTS

### N(1710) $P_{11}$ resonant state is finally confirmed

Using the multi-channel, multi-resonance coupled-channel partial wave analysis developed entirely in the Division of Experimental Physics. It has been shown that the controversial N(1710)  $P_{11}$  resonant state definitely exists when the data in inelastic channels

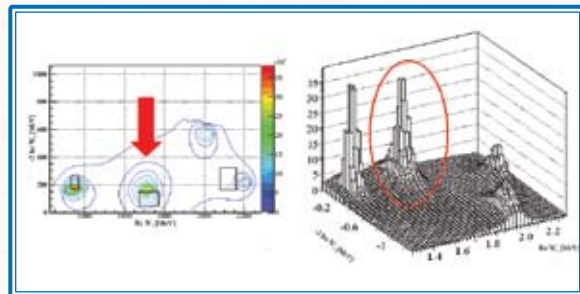


Figure 1: N(1710)  $P_{11}$  resonant state.



are systematically included. If only elastic channel is used, the answer is ambiguous. This is a first step in overall application of the existing multi-channel code in hadron spectroscopy with the aim to re-evaluate the confidence level of all low lying nucleon resonant states (Ceci et al., Phys Rev Lett 2006: 97: 062002-1).

### Exotic nuclear structure and reaction

The 10.15 MeV resonance in  $^{10}\text{Be}$  has been probed via resonant  $^6\text{He}+^4\text{He}$  elastic scattering. It was unambiguously demonstrated that the state has spin and parity  $4^+$  and a very large reduced width for  $\alpha$ -particle decay. The results confirm our previous suggestions and findings that it is the third member of a rotational band based on the 6.18 MeV  $0^+$  state. It's extremely large deformation, together with a significant degree of clusterization, signals an exotic, well developed  $\alpha : 2n : \alpha$  molecular structure.

Another interesting result (in addition to those previously published) surfaced from the analysis of data from the measurement of the  $^6\text{He}+^6\text{Li}$  reactions. Evidence was found on the  $^6\text{He}$  quasi-free scattering on deuteron clusters in  $^6\text{Li}$  nucleus at energy of

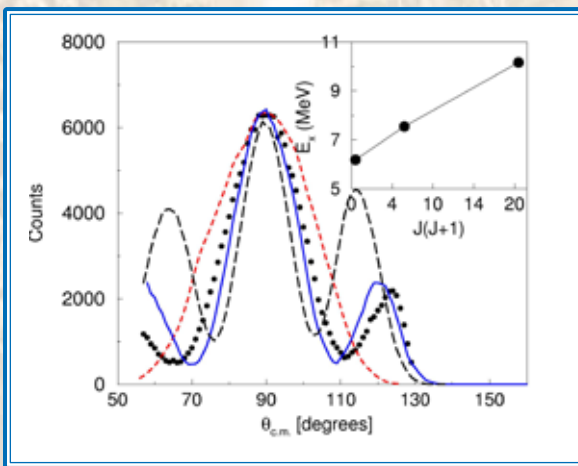


Figure 2: Experimentally determined centre-of-mass distribution compared with simulations for the decay of a spin 2, 4 and 6 resonance.

$^6\text{He}$  projectiles of only 18 MeV. This is the first observation of the quasi-free scattering of loosely bound, «fragile» radioactive nuclei on clusters in target nuclei. (Miljanić Đ et al., Europhys Lett 2006: 76:801).

### Neutrino dark energy

We have shown that a simple coupled system of a variable vacuum term and a gas of relic neutrinos may account not only for the correct amount of dark energy at present, but also for a near coincidence between the matter and dark-energy densities to hold over a significant portion of the history of the universe (Horvat R, J Cosmol Astropart Phys 2006: 01: 015).

### Proton-proton bremsstrahlung

In collaboration with the KVI, Groningen a series of nucleon-nucleon bremsstrahlung experiments at 190 MeV incident beam en-

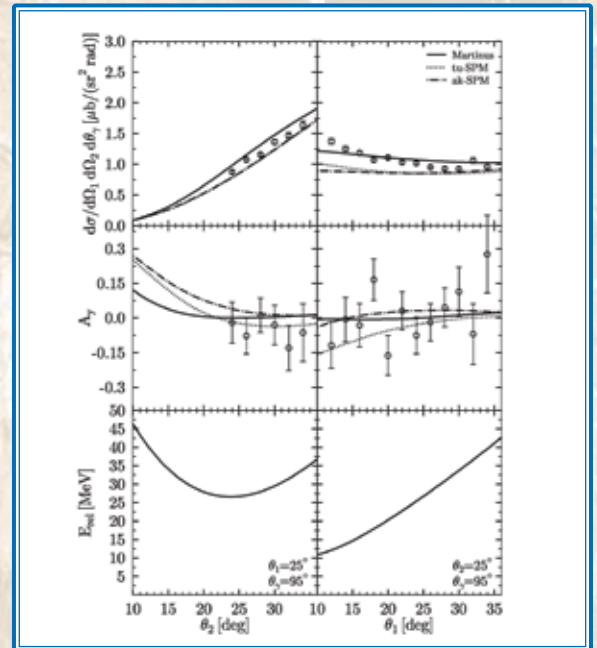


Figure 3: Cross sections, analyzing powers, and relative energies, for the combination  $\theta_1(\theta_2) = 25^\circ$ ,  $\theta_\gamma = 95^\circ$  in the left (right) panel as a function of  $\theta_2(\theta_1)$ . Only statistical errors are shown here. The solid, dotted and dash-dotted curves are the predictions of the microscopic model and of the two different soft-photon models, respectively.

ergy have been performed in order to gain more insight into the dynamics governing the bremsstrahlung reaction. After initial measurements wherein the bremsstrahlung process was studied far away from the elastic limit, a new study was carried out to probe the process nearer to the elastic limit. Measured cross sections and analyzing powers are compared with the predictions of a microscopic model and those of two soft-photon models. For some kinematics the theoretical calculations overestimate the data by up to approximately 30%, indicating that a subtle refinement of the current theoretical models is required. The analysis of the higher order i.e. two-photon and virtual (emission of the electron-positron pair) bremsstrahlung measurements is in progress. (Mahjour-Shafiei et al., Phys Lett B 2006: 632: 480).

### Experimental High Energy Physics

Transverse mass spectra and rapidity distributions of strange particles were studied in the beam energy range 20A -158A GeV with the NA49 large acceptance detector at the CERN-SPS. The measurements of the  $\Lambda$  and  $\Xi$  hyperon enhancement factors are shown for the first time. Results are obtained for energy and centrality dependence of antiproton production in Pb+Pb collisions in the same energy range. High transverse momentum spectra, up to 4 GeV/c, of identified particles produced in Pb+Pb collisions at 158 A/GeV beam energy, are used to extract the nuclear modification factor for pions, kaons and protons, and the study of baryon to meson ratios. New results on the production of charged pions in p+p interactions at 158 GeV/c are presented. Inclusive invariant cross sections are given over the interval from 0 to 2 GeV/c in transverse momentum and 0 to 0.85 in Feynman x (Alt C et al., Eur Phys J C 2006: 45: 343).

### OPERA neutrino oscillations experiment

Scientists from our Laboratory for Electromagnetic and Weak Interactions are involved in the OPERA long-baseline experiment designed to investigate neutrino oscillations. Our group works on the development and testing of the GRPC detector for veto system of the OPERA detector, which is placed at the underground Gran Sasso Laboratory, 732 km away from the CERN neutrino source. In August 2006 a first test-run with CERN-to-Gran Sasso neutrinos was successfully conducted. The first events from the CNGS neutrino beam were taken in 2006. (Acquafredda R et al., RBI-OPERA collaboration (K. Jakovčić, A. Ljubičić, M. Stipčević) New J Phys 2006: 8: 303).



Figure 4: OPERA experimental set-up.

### K $\beta$ x-ray spectra of vanadium compounds

K $\beta$  x-ray spectra of metallic vanadium and selected compounds induced in thick targets by 3 MeV proton beams were measured by using a wavelength dispersive x-ray spectrometer installed at the RBI Tandem Accelerator facility. In addition to the main K $\beta_{1,3}$  x-ray line, second order contributions like K $\beta'$ , K $\beta''$ , K $\beta'''$  and K $\beta_{2,5}$  were clearly resolved. It has been observed that the intensities and positions of these lines relative to the K $\beta_{1,3}$  x-ray line are influenced



by the oxidation states of vanadium in studied compounds. The obtained results indicate that the strength of the  $K\beta''$  and  $K\beta_{2,5}$  transition probability per vanadium-ligand pair decreases exponentially with increasing vanadium-ligand distance, which is in agreement with an earlier observation reported by other authors for  $K\beta''$  relative intensity in a number of Mn oxide compounds (Fazinić S et al., Phys Rev A 2006: 74: 062501).

## NEW EQUIPMENT

### Helicity Dependence pion Photoproduction and the GDH integral on the neutron

To measure the spin structure of the nucleons, both a polarized beam and a polarized target are required. Some such measurements have already been performed. However due to technical difficulty, the measurements of the so called "GDH Sum Rule" have been performed only recently. Therefore, the developments of the longitudinally polarized target, as well as the technically more challenging transversally polarized target, are underway at MAMI, Mainz. Specifically, the frozen spin polarized target is the most appropriate for our experimental program. To acquire physical data, exact knowledge of polarization is crucial and measurement using continuous wave nuclear magnetic resonance (NMR) technique is best suited for that purpose. The heart of this apparatus is the so called NMR module which is jointly developed by scientists from Universities of Mainz and Bochum and from the Rudjer Bošković Institute. A significant part of that setup will be assembled and tested at RBI.

### CMS High Level Trigger

We have finished and implemented the design of an expert system-based problem solver for the CMS Event Filter farm and integrated it in the Run control software of the CMS Trigger and Data Acquisition system, and have started to test

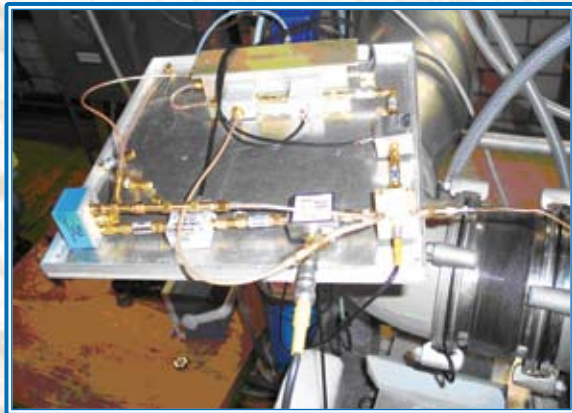


Figure 5: NMR test setup for measurement of polarization of the frozen spin target.

its performance. We have also started to work on the electron-muon filter in the CMS High Level Trigger. We have developed a selection for WZ diboson production which will be used to measure triple gauge boson couplings. Our analysis has shown that this process can be measured very early in the LHC run with a high signal to background ratio.

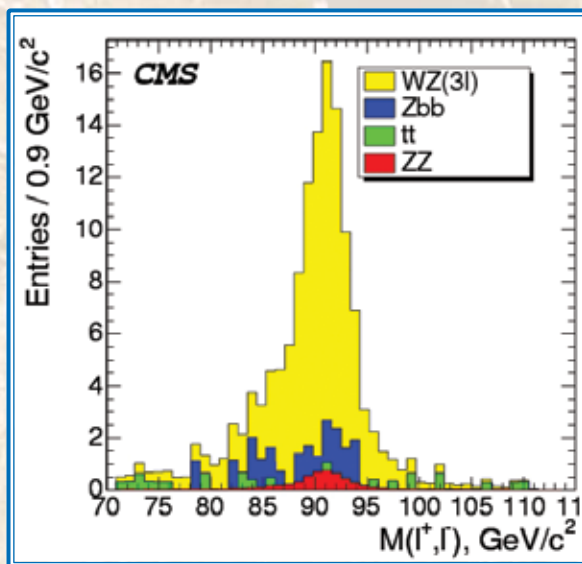


Figure 6: Reconstructed Z boson invariant mass for simulated  $pp \rightarrow WZ$  events. The yellow histogram shows the signal contribution while the background contributions are shown in other colours after all selection criteria have been applied.



## Cooperation with Croatian Conservation Institute

Carbon dating and particle induced x-ray emission (PIXE) spectroscopy of samples from cultural heritage objects have been for many years the basis of collaboration with Croatian Conservation Institute (CCI). Under the IAEA technical cooperation project, analytical capabilities of both Institutes have been upgraded. New mobile XRF system has been provided for CCI, while the construction of new in-air PIXE beam line and upgrade of ion microprobe has been completed at RBI. Recent joint projects include characterization of the Apoxiomenos statue and analysis of pigments in paintings of Master HGG. Both projects resulted in exhibitions presented to the public in 2006.



Figure 7: Elemental analysis of Apoxiomenos sculpture performed by using PIXE spectroscopy at the new in-air beam line of the 1.0 MV Tandemtron accelerator.

## Methods of explosive, chemical and nuclear material detection

The project consists of R&D investigations of the application of neutron technology to the inspections of sea containers for the control of illicit trafficking of threatening materials such as explosives and nuclear material. The technology chosen for the research applies the so-called "associated particle technique", which provides beams of tagged neutrons able to pin down a well defined region inside the container where the inspection is being made. The research activity involves the design, construction and testing of neutron generators, alpha particle detectors,

gamma-ray detectors, neutron counters and related electronics and data acquisition systems.

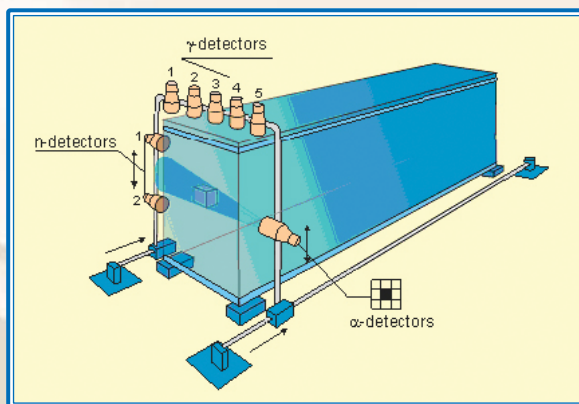


Figure 8: Neutron sensor incorporating neutron source, gamma and neutron detectors.

## Natural isotopes in environmental studies and radiocarbon dating

A new line for benzene synthesis for  $^{14}\text{C}$  activity measurements in very small samples is under construction, and the construction of the system for preparation of samples to be measured by AMS technique is in progress.

## EDUCATION

A number of scientists from the Division of Experimental Physics have continued to maintain a significant educational activity at undergraduate and graduate studies of University of Zagreb, University of Rijeka and University of Dubrovnik.

## PROJECTS

### Projects supported by the Ministry of Science, Education and Sports

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

### **Research, developmental and international projects**

1. Nuclear techniques for the analysis and preservation of national heritage objects, Milko Jakšić (IAEA Technical Co-operation project, Res. Contract CRO/1/005)
2. Study of advantages and limitations of Si pin diodes as radiation detectors by ion beam methods, Milko Jakšić (bilateral project with Hungary)
3. Measurements of differential cross sections for elastic scattering of  $^1\text{H}$  and  $^4\text{He}$  ions from selected light elements, Ivančica Bogdanović Radović (IAEA Research Contract 13269/RO)
4. Heavy ion acceleration in 1.0 and 6.0 MV electrostatic accelerators, Milko Jakšić (IAEA Research Contract 13127/RO)
5. Upgrade of PIXE and STIM imaging capabilities at Zagreb nuclear microprobe, Mladen Bogovac (IAEA Research Contract 13258/RO)
6. Characterization of inorganic pigments used by selected painter(s) by nuclear microprobe, Stjepko Fazinić (IAEA Research Contract 13050/RO)
7. Modification of electronic properties in insulators using nuclear microprobe, Zvonko Medunić (IAEA Research Contract 12925/RO)
8. European Commission Framework Program 6 Project EUROpean Nuclear Structure Integrated Infrastructure Initiative – EURONS, Zoran Basrak (EC Contract 506065)
9. Heavy ion physics, International collaboration project RBI-KFKI Research Institute for Particle and Nuclear Physics, Budapest via Croatian (HAZU) and Hungarian Academy of

- Science, Roman Čaplar
10. Investigation of influence of forest ecosystems of National Park Plitvice to the quality of water and lakes, Nada Horvatinčić (National Park Plitvice research project).
11. Application of isotope techniques in investigation of water resources and water protection in the Karst area of Croatia, Nada Horvatinčić, In co-operation with the University of Rijeka, Dept. of Physics of the Faculty of Medicine. (IAEA Technical co-operation programme CRO/8/006)
12. Control of illicit trafficking in threat materials and humans, Vladivoj Valković (NATO project No. SfP 980526)
13. EURITRACK, European illicit trafficking countermeasures kit, Vladivoj Valković (EU FP6 Specific Targeted Research or Innovation Project No. 511471)
14. Elastic scattering of electrons and positrons, Ines Krajcar Bronić, In co-operation with the International Commission on Radiation Units and Measurements, Bethesda, MD, USA (ICRU 77)
15. International collaboration between RBI and LNS, Catania, Italy on investigation of binary dissipative processes around the Fermi energy, Zoran Basrak
16. International collaboration between RBI and GSI, Darmstadt, Germany on investigation of nuclear equation of state, Roman Čaplar
17. International collaboration between RBI and KVI, Groningen, The Netherlands on investigation of virtual and double photon bremsstrahlung, Roman Čaplar
18. International collaboration between RBI and INFN-LNL, Legnaro (Padova), Italy on investigation of properties of nuclear surface, Suzana Szilner
19. International collaboration between RBI and MAMI, University of Mainz, Germany on development of frozen spin polarization target, Ivan Supek
20. International collaboration between RBI and University of Virginia, USA on PIBETA experiment, Ivan Supek
21. International collaboration between RBI and CERN, Geneva, Switzerland on CERN Axion Solar Telescope (CAST) experiment, Milica Krčmar
22. International collaboration between RBI and CERN, Geneva, Switzerland in ALICE, Tome



Antičić; CMS, Krešo Kadija and NA49 collaborations, Krešo Kadija

23. International collaboration between RBI and CERN, Geneva, Switzerland on NOMAD collaboration, Ante Ljubičić
24. International collaboration between RBI, CERN (Geneva, Switzerland) and LNGS (Gran Sasso, Italy) on OPERA collaboration, Ante Ljubičić

## SELECTED INVITED LECTURES

1. Brigljević V: Measurement of di-boson production with CMS, Physics at LHC, Krakow, Poland, July 3-8, 2006.
2. Fazinić S: Accelerator Techniques for Cultural Heritage in Croatia, International Workshop for Science in Cultural Heritage, Trieste, Italy, October 23-28, 2006.
3. Jakšić M: Characterization of materials and radiation damage induced changes using heavy ion beams, NIS Coloquium: Micro-analysis and micromodification of materials by ion beams, Torino, Italy, December 18-20, 2006.
4. Kadija K: Towards the 3-D imaging of the collision region on the femtometer scale, 10th International Brijuni Conference: Imaging in space and time, Brijuni, Croatia, August 28 – September 1, 2006.
5. Sudac D: Identification of materials hidden inside a container by using the 14 MeV tagged neutron beam, 19th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas, USA, August, 20-25, 2006.
6. Szilner S: Binary Reactions Explored with Prisma + Clara, IX International Conference on Nucleus-Nucleus Collisions (NN2006). Rio de Janeiro, Brazil, August 28 - September 1, 2006.
7. Šlaus I: Few-Body Research – Summary. 18th International IUPAP Conference on Few-Body Problems in Physics, Santos, Brazil, August 21-26, 2006.

## SELECTED ORGANIZED CONFERENCES

1. International Conference on Reaction Mechanisms and Nuclear Structure at the Coulomb Barrier, San Servolo, Venice, Italy, March 19-23, 2006.

## SELECTED PUBLICATIONS

1. Ceci S, Švarc A, Zauner, B:  $\pi N \rightarrow \eta N$  data demand the existence of  $N(1710) P_{11}$  resonance reducing the 1700 MeV continuum ambiguity. Phys Rev Lett 2006: 97: 062002-1.
2. Freer M, et al. (Milin M, Soić, N): molecular bond in  $^{10}\text{Be}$ , Phys Rev Lett 2006: 96:042501.
3. Horvat R: Mass-varying neutrinos from a variable cosmological constant. J Cosmol Astropart Phys 2006: 01: 015.
4. Mahjour-Shafiei M, et al. (SALAD Collaboration-IRB : Gašparić I, Kiš M): Proton-proton bremsstrahlung towards the elastic limit at 190 MeV incident beam energy. Phys Lett B 2006: 632: 480.
5. Marginean N, et al. (PRISMA Collaboration-IRB : Szilner S): Shape transitions far from stability: The nucleus  $^{58}\text{Cr}$ . Phys Lett B 2006: 633: 696.
6. Alt C, et al. (NA49 Collaboration-IRB: Antičić T, Kadija K, Nikolić, V, Šuša T): Upper limit of  $D^0$  production in central Pb-Pb collisions at 158 AGeV, Phys Rev C 2006: 73: 034910-1.
7. Acquafredda R, et al. (RBI-OPERA collaboration: Jakovčić K, Ljubičić A, Mićanović S, Stipčević M, Zamboni I): First events from the CNGS neutrino beam detected in the OPERA experiment. New J Phys 2006: 8: 303.
8. Alt C, et al. (NA49 Collaboration-IRB: Antičić T, Kadija K, Nikolić V, Šuša T): Inclusive production of charged pions in p+p collisions at 158 GeV/c beam momentum, Eur Phys J C 2006: 45: 343.



9. Fazinić S, Jakšić M, Mandić L, Dobrinić J: Chemical dependence of second order radiative contributions in the  $K\beta$  X-ray spectra of vanadium and its compounds, *Phys Rev A* 2006: 74: 062501.
10. Miljanić Đ, Milin, M, Cherubini S; Davinson T, DiPietro A, Figuera P, Musumarra A, Ostrowski AN, Pellegriti MG, Shotton AC, Soić N, Spitaleri C and Zadro M:  $^6\text{He}$  quasi-free scattering off clusters in  $^6\text{Li}$ . *Europhys Lett* 2006: 76:801.
11. Szilner S, Haas F, Basrak Z, Freeman RM, Morsad A and Nicoli MP: Competition between direct and dissipative processes in the binary channels of the  $^{16}\text{O}+^{12}\text{C}$  and  $^{18}\text{O}+^{12}\text{C}$  reactions. *Nucl Phys A* 2006: 779: 21.

## Chapters in books

1. Sironić A, Markuš M, Marković B: New additive for alcohol free dampening In: *Graphic arts: technology, design, communications*. University Press, Faculty of Graphic Arts Zagreb, 2006 pp 149-156.
2. Krajcar Bronić I: Physical dating methods in archaeology and art, In: *This is physics too*, Croatian Physical Society Press, Zagreb 2006 pp. 69-77.
3. Ivezić T: Lorentz invariant Majorana formulation of the field equations and Dirac-like equation for the free photon. *Majorana legacy in contemporary physics*. Di Renzo Press, Rome, Italy, 2006 pp 131-142.

# Division of Materials Physics

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

## DIVISIONAL ORGANIZATION

Head: Nikola Radić

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 which describe and connect the microscopic, mesoscopic and macroscopic properties of condensed matter and molecules. 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.

Nanoscience and nanotechnology has been the most active direction of both fundamental scientific research and developments in technology for the Division of Materials Physics. Various types of nanostructured materials have been produced: amorphous

and nanocrystalline thin films produced by thermodynamically non-equilibrium processing (magnetron sputtering, ion implantation), particularly Al-based amorphous alloys, a-Si and a-Si<sub>1-x</sub>C<sub>x</sub>:H films, nanolaminates of semiconductor (Ge, Si)/ dielectric (SiO<sub>2</sub>) bilayers - as precursors for nanoparticles, nanocrystalline metals (nc-Ni), nanosized ceramics (ZrTiO<sub>4</sub>) and nanocomposites (CeVO<sub>4</sub>). The structure of these materials has been examined by different methods - XRD, SAXS, Raman spectroscopy, electron microscopy etc., and physical properties were correlated with the respective findings.

The Division 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.

Finally, the optical interactions in matter in the strongly nonlinear range, and the spontaneous and induced self organization in condensed systems are the subject of intensive research.



## TOP ACHIEVEMENTS

### Selected results in study of glass implanted with gold ions.

The interest in metal nanocrystals is focused on their nonlinear optical properties, as they are expected to have a large third order nonlinear susceptibility. In order to explore the possibility of tuning the size and shape of metal nanocrystals we implanted gold into fused silica substrate. Grazing incidence small-angle X-ray scattering (GISAXS) was used to study the morphology and the distribution of gold nanoparticles formed in the substrate. Upon annealing, the number of clusters, as well as their size is increased. At the highest annealing temperature the clustering diverges into two distinct size distributions (Pivac B et al., Scripta Materialia 2006: 55: 135).

### Temperature evolution in nanostructured $\text{CeVO}_4$ films

Cerium vanadate films on glass substrate were obtained by the sol-gel process. The morphology of these nanostructured and porous films was studied by grazing-incidence small-angle X-ray scattering (GISAXS) at

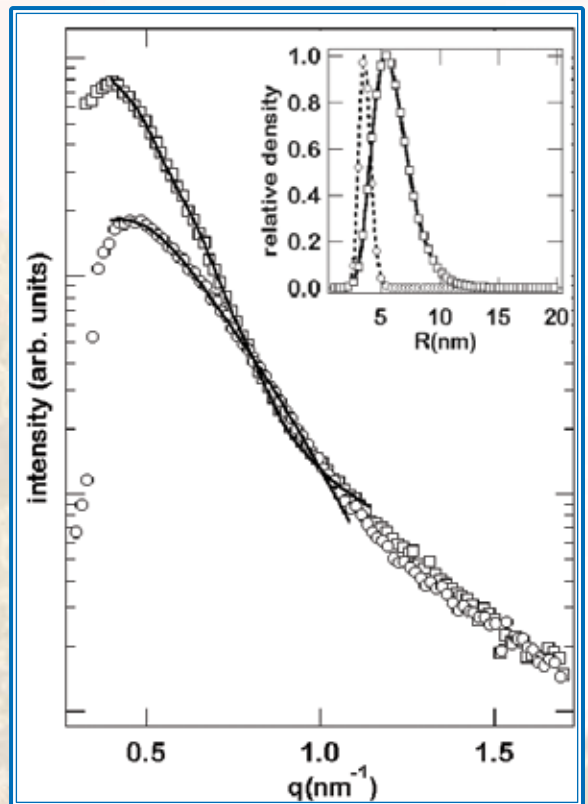


Figure 1: GISAXS intensities vs. scattering angle for the  $6 \times 10^{16}$  ions/cm<sup>2</sup> dose implanted sample, annealed at 1000°C (circles) and 1100°C (squares).

the synchrotron ELETTRA, Trieste, Italy. The aim of the GISAXS study was to investigate the changes in grain sizes due to the tem-

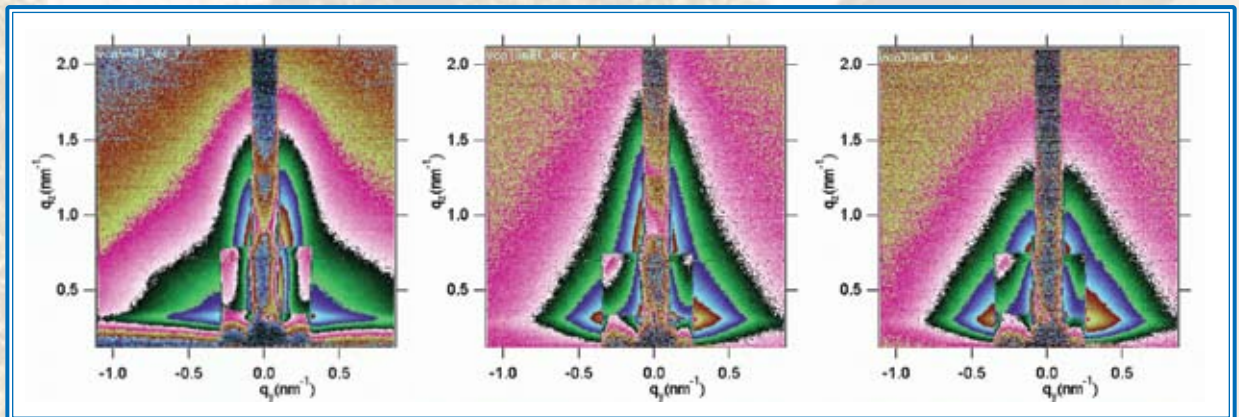


Figure 2a

Figure 2b

Figure 2c

Figures 2a-c: 2-D GISAXS patterns of V/Ce oxide with different annealing times. Although the increase in size is common to all the samples, it is far more pronounced in the bulk. The result is that for short annealing time grain sizes are bigger close to the surface, while this is reversed after long annealing. Average grain radii obtained from fit in linear vertical cut are:  $\langle R \rangle = 2.5$  nm, 3.0 nm and 3.1 nm, respectively.



perature evolution with three different time intervals (5min., 15 min. and 30 min.) of annealing at 673 K. It was found that the effects of the different annealing times are different for the surface and the bulk properties of this V/Ce oxide (Turković A et al., J Electrochem Soc 2006: 153: A122)

### Sputter deposited nanocrystalline Ni and Ni-W films as catalysts for hydrogen evolution

Nanocrystalline nickel (nc-Ni) and Ni-W alloy coatings have been prepared by the dc magnetron sputtering deposition method, and their catalytic properties for the hydrogen evolution reaction (HER) were investigated in an alkaline electrolyte solution. The kinetic parameters deduced from linear polarization and electrochemical impedance spectroscopy measurements indicated outstandingly high electrocatalytic activity of Ni-W and nc-Ni films. The best performance toward the HER demonstrates the Ni<sub>90</sub>W<sub>10</sub> alloy in accordance with the prediction based on the electronic structure calculations and the enhanced density of states at the Fermi level of the 3d Ni band (Metikoš-Huković M et al., J Mol Catalysis A: Chemical 2006: 249: 172).

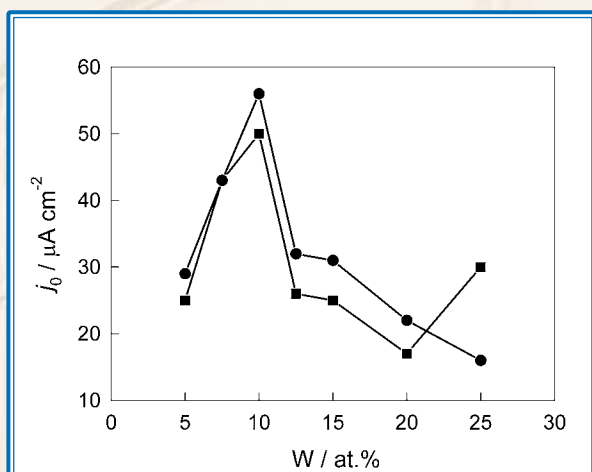


Figure 3: The dependence of the exchange current density,  $j_0$  obtained from EIS (●) and polarization (■) measurements, on the content of W in the coating.

### Low Frequency Raman Scattering of Nanoparticles and Nanocomposite Materials

The particle-size distributions determined by Raman scattering were compared to these found by TEM measurements. Raman spectroscopy proves to be a simple, fast and reliable method for size-distribution measurements. By an inverse procedure, starting from the Raman spectra and known particle-size distribution, a new method for the determination of the mean sound velocities of longitudinal and transverse phonons of nanoparticles is described (Ivanda M et al., J Raman Spectr 2006: 37: 161).

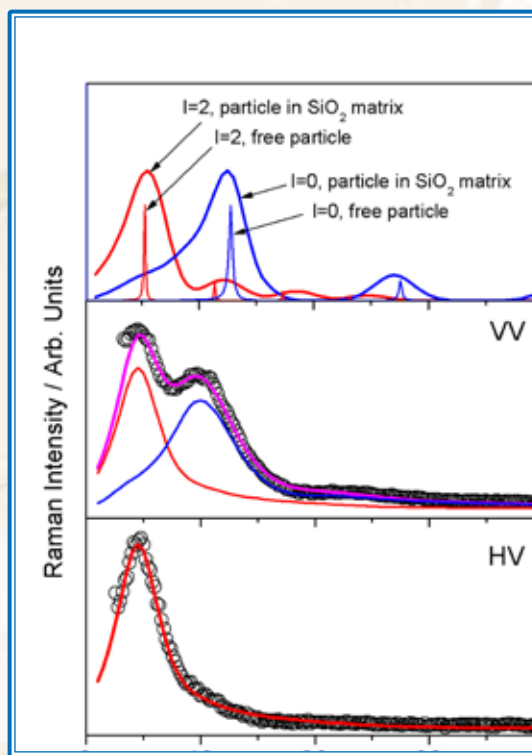


Figure 4: The calculated symmetric and quadrupolar Raman peaks of the free anatase particle of 20.8 nm in diameter (sharp lines) and of the same particle in SiO<sub>2</sub> matrix (solid lines); b) fit of the symmetric and quadrupolar modes on the VV polarized Raman spectrum with the size distribution obtained from the TEM, c) the same fit for the quadrupolar mode in the HV Raman spectrum. The fit gives the value of longitudinal and transverse sound velocity of anatase:  $v_l = 8880$  m/s, and  $v_t = 3900$  m/s.

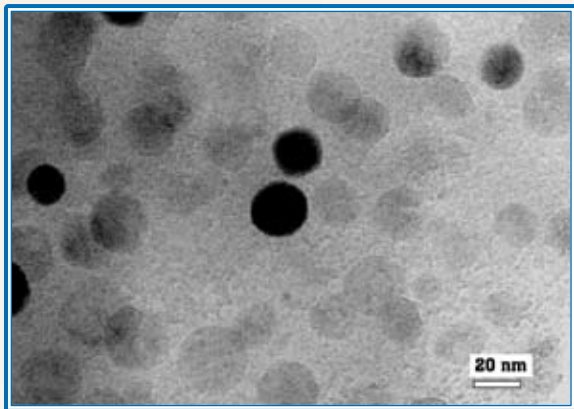


Figure 5: TEM image of a sol-gel  $0.8\text{SiO}_2-0.2\text{TiO}_2$  film heated at  $1300^\circ\text{C}$  showing anatase crystals in a glass matrix with Gaussian distribution of mean size  $D_0=20.8\text{ nm}$  and  $\sigma=3.18\text{ nm}$ .

## NEW EQUIPMENT

### Molecular Physics Laboratory - A new Raman spectrometer installed

A new Raman spectrometer, T64000 from HORIBA-Jobin Yvon, was purchased and installed in Molecular Physics Laboratory in December of 2006. With its high, research oriented flexibility, it will promote the materials science at the Ruđer Bošković Institute and in Croatia as a whole. Detection of scattered light crucial for Raman spectroscopy is now enhanced by alternative use of two CCD detectors, covering spectral region from UV to NIR. Thus, previously inaccessible samples such as opaque or sensitive materials can be studied using smaller laser power at the focus, while the recording time is greatly



Figure 6: A new T64000 HORIBA-Jobin Yvon Raman spectrometer in Molecular Physics Laboratory.

reduced for others. The system includes microscope with automated XY stage, onto which a variable temperature cell (90 K – 600 K) can be mounted. In this way one can record spectra for a chosen sample surface and analyze the surface composition and temperature changes.

## PROJECTS

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

1. Impact of Defects and Nanostructures on Semiconductor Properties, Branko Pivac
2. Magnetron Deposition of Thin Films, Nikola Radić
3. Physics and Application of Nanostructures, Krešimir Furić
4. Multiphase Amorphous Silicon Alloys as Thin Films, Davor Gracin
5. Sugar Hydration Dynamics, Vlasta Mohaček-Grošev
6. Nanophase Films and Nanocomposite Solid Electrolytes Research, Aleksandra Turković
7. Static and Dynamics of Molecular Solids, Davor Kirin
8. Optical Interactions and Organizational Processes in Matter, Stjepan Lugomer
9. Semiconductor Materials for Optoelectronics, Branko Šantić
10. Influence of dopands on the structure and properties of materials for technical applications, Biserka Gržeta

### Research, development and international projects

1. Study of nanocomposite polymer electrolytes, Aleksandra Turković (Bilateral collaboration with Slovenia)
2. Study of disordered materials, nano-optical layers, Mile Ivanda (Bilateral collaboration with Slovenia)
3. Research on silicon and germanium nanostructures, Branko Pivac (COGITO - Bilateral collaboration with France)
4. LPMAS, Davor Gracin (EU- FW6 -INCO- Project No FP6-509178)
5. RISE, Uroš V. Desnica (EU-FW6-INCO- Project No FP6-509161)



- Hybrid photovoltaic module, Davor Gracin (Ministry of Science, Education and Sport-HITRA-STIRP Project TP-02/0098-35)

## INVITED LECTURES

Popović J: Defect structure examination of Sn-doped indium oxide (ITO). 10th European Powder Diffraction Conference, Geneva, Switzerland, September 1-4, 2006.

## SELECTED ORGANIZED CONFERENCES

The 13th International Meeting "Vacuum Science and Technique", Koprivnica, June 13, 2006, was organized by the Division members N. Radić, B. Pivac, I. Capan and T. Car on behalf of the Croatian Vacuum Society.

The 50<sup>th</sup> IUVSTA workshop "Toward Novel Nanostructure-based Devices: Nanostructured materials fabrication, characterization and assembly for novel devices", 22-27 October 2006, Dubrovnik, has been co-organized by the Rudjer Bošković Institute. Branko Pivac was the International Program Committee Chair, while B. Pivac and N. Radić were members of the Local Organizing Committee ([www.nano2006.org/download](http://www.nano2006.org/download)).

## SELECTED PUBLICATIONS

- Delgado J, Su D, Rebmann G, Keller N, Gajović A, Schlögl R: Immobilized carbon nanofibers as industrial catalyst for ODH reactions. *J Catalysis* 2006: 244: 126.
- Lugomer S, Maksimović A, Peto G, Toth A, Horvath E: One-Dimensional and Two-Dimensional Array of Nanoholes Generated by Laser -Matter Interaction in the Semiconfined



Figure 7: The 13th International Meeting "Vacuum Science and Technique" and The 50<sup>th</sup> IUVSTA workshop "Toward Novel Nano-structure-based Devices: Nanostructured materials fabrication, characterization and assembly for novel devices".



- Configuration. J Appl Physics 2006: 100: 4308.
3. Metikoš-Huković M, Grubač Z, Radić N, Tonejc A: Sputter Deposited Nanocrystalline Ni and Ni-W Films as Catalysts for Hydrogen Evolution. J Mol Catalysis A: Chemical 2006: 249: 172.
  4. Pivac B, Dubček P, Kovačević I, Bernstorff S, Mu R, Wu M, Ueda A, Vlahović B: GISAXS study of gold implanted fused silica. Scripta Materialia 2006: 55: 135.
  5. Risović D: Interfacial adsorption with molecular reorientation. J Electroanal Chem 2006: 588: 122.
  6. Turković A, Pavlović M, Ivanda M, Gaberšček M, Crnjak Orel Z: Influence of Intercalated Lithium on Structural and Electrical Properties of  $V_2O_5$ , Mixed V/Ce Oxide and  $Fe_2O_3$ . J Electrochem Soc 2006: 153: A122.
  7. Gradišnik V, Pavlović M, Pivac B, Zulim I: Transient Response Times of a-Si:H p-i-n Color Detector. IEEE Trans Electron Dev 2006: 53: 2485.
  8. Ivanda M, Hohl A, Montagna M, Mariotto G, Ferrari M, Crnjak Orel Z, Turković A, Furić K: Raman Scattering of Acoustical Modes of Silicon Nanoparticles Embedded in Silica Matrix. J Raman Spectr 2006: 37: 161.

## DIVISIONAL ORGANIZATION

Head of department: Hrvoje Zorc

The Division of Laser and Atomic R&D consists of the following laboratories:

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



## TOP ACHIEVEMENTS

### Optical thin films

The characterization of layers that are mixtures of two materials using different effective medium approximations has been done. Besides modelling the refractive index of materials, extinction coefficients of the mixtures have also been studied. Optical characterization of hybrid antireflective coatings combining spectrophotometric and ellipsometric measurements have been successfully performed, indicating possible weak points of the deposition processes by which the rugate structures have been deposited. (Leitel R et al., Thin Solid Films 2006: 497: 135).

### Colour detection

In the field of colour detection using a-Si: H p-i-n detector a new method is proposed where „on“ and „off“ response times of light pulse are being used. It has been shown that, depending on type of illumination and pulse one or two different mechanisms con-

## OVERVIEW OF THE DIVISION

The mission of the Division is to expand and strengthen the knowledge in the field of imaging and non-imaging optics and on the optical thin film fundamentals. Besides that activities are directed to the application of these basic disciplines in the fields of medicine and national security.

The Division is currently developing several strategic projects. These include the development in the medical field, particularly the new technologies and techniques for photodynamic diagnostics and therapy of skin malignant diseases. A significant step forward has been made in introducing blind signal deconvolution in the field of photodynamic diagnosis.



tribute to conductivity. Both include capture and emission from deep and shallow traps for both types of charge carriers. Characteristic transients of photo currents and response times have high potential in colour recognition and enable further development towards artificial vision (Gradišnik V et al., IEEE Trans EI Dev 2006: 53: 2484).

### Blind signal processing

In the field of blind signal and image deconvolution the following novel approaches have been developed: a wavelet-packets-based approach to the blind separation of statistically dependent sources, unsupervised segmentation of low-dimensional multispectral images combining a nonlinear band generation process and the blind separation of statistically dependent sources, and a new constrained-kurtosis maximization approach to unsupervised segmentation of high-dimensional hyperspectral data (Huang TM et al., Studies in Computational Intelligence 2006: 17).

### Photodynamic diagnosis and therapy

One of the major achievements in 2006 was development and testing of an advanced apparatus for photodynamic diagnosis and therapy (PDT and PDD) of skin malignant diseases under the brand name - MediLED-7®. The device is going to be completed with new software in 2007.

### PATENT APPLICATION

In 2006 a new patent application has been submitted.

1. HR2006/P20060149A Intelligent portable contact illuminator for photodynamic therapy of surface tumors

## PROJECTS

### Basic research project supported by the Ministry of Science, Education and Sports:

1. Photonics of imaging and non-imaging optical systems, Hrvoje Zorc

### Research and development projects supported by the Ministry of Science, Education and Sport

1. Detection of skin tumours by fluorescence of exogenous protoporphyrin IX (PpIX), Anton Peršin (HITRA-TEST)

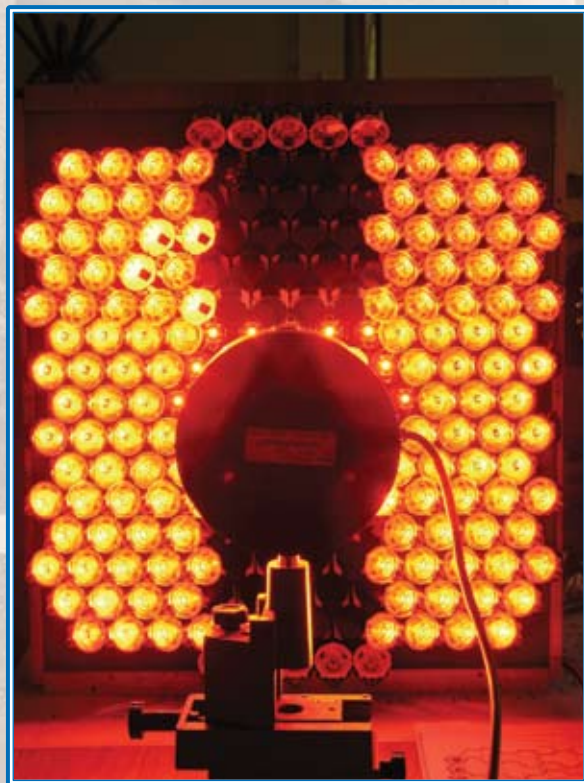


Figure 1: Apparatus for photodynamic diagnosis and therapy of skin malignant diseases.



## In-House research and development projects:

1. Development of night vision systems
2. Development of multicomponent optical systems

## SELECTED PUBLICATIONS:

1. Leitel R, Stenzel O, Wilbrandt S, Gäbler D, Janicki V, Kaiser N: Optical and non-optical characterization of  $\text{Nb}_2\text{O}_5\text{-SiO}_2$  compositional gradient index layers and rugate structures. *Thin Solid Films* 2006: 497: 135.
2. Janicki V, Gäbler D, Wilbrandt S, Leitel R, Stenzel O, Lappschies M, Görtz B, Ristau D, Rickers C, Vergöhl M: Deposition and spectral performance of an inhomogeneous broadband wide-angular antireflective coating. *Appl Opt* 2006: 45: 7851.
3. Gradišnik V, Pavlović M, Pivac B, Zulim I: Transient response times of a-Si:H p-i-n color detector. *IEEE Trans El Dev* 2006: 53: 2484.
4. Turković A, Pavlović M, Ivanda M, Gaberšček M, Crnjak Orel Z: Influence of intercalated Lithium on structural and electrical properties of  $\text{V}_2\text{O}_5$ , mixed V/Ce oxide and  $\text{Fe}_2\text{O}_3$ . *J Electrochem Soc* 2006: 153: A122.
5. Kopriva I, Garrood D J, Borjanović V: Single frame blind image deconvolution by non-negative sparse matrix factorization. *Opt Comm* 2006: 266: 456.
6. Abdallah H, Wasyliwskyj W, Kopriva I: Equalization of numerically calculated element radiation patterns for root-based direction finding algorithms. *ACES J* 2006: 21: 76.
7. Du Q, Kopriva I, Szu H: Independent component analysis for hyperspectral remote sensing. *Opt Eng* 2006: 45: 17008.

## Books

1. Huang T M, Kecman V, Kopriva I, Kernel based algorithms for mining huge data sets: supervised, semi-supervised and unsupervised learning. *Springer Series: Studies in Computational Intelligence* 2006: 17.

## CERTIFICATES

In 2006 the Division received the ISO 9001:2000 certificate.



Figure 2: ISO 9001:2000 certificate.





# Division of Electronics

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

## DIVISIONAL ORGANIZATION

Head: Tomislav Šmuc

The Division of Electronics consists of the following laboratories:

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



## TOP ACHIEVEMENTS

### Machine learning and data mining research

The main developments in this area were concentrated on techniques that foster either descriptive or predictive capabilities of existing methods such as subgroup discovery, SVM, Parallel Random Forests in combination with diverse feature construction and filtering methods. An enhanced machine learning methodology for the analysis of 1D electrophoresis experiments has been developed and applied for plant tissue discrimination. Machine learning models based on the support vector regression technique and self-organizing-maps were developed for the prediction of the mechanism of action and assessment of the antitumour potential of a new class of chemical entities, based on biological responses from in-vitro experiments. Applications of optimized methodologies range from molecular biology (Gamberger D et al., Inform Med Slov 2006: 11: 46), drug-discovery to information processing and retrieval and engineering.

## OVERVIEW OF THE DIVISION

The Division of Electronics continues to work on research and development of novel intelligent data and signal analysis techniques, and their application in areas of highest scientific interest such as: biomedicine, computational biology and bioinformatics, as well as on development of advanced measurement and signal processing systems. With the start of the 6th European Framework STREP project HEARTFAID, the Laboratory for information systems initiated research in knowledge engineering, primarily focused on knowledge representation and management in the field of heart failure disease. Laboratory for stochastic signals and processes research is continuing development of measurement methodology and data acquisition protocols for human locomotion and human jaw kinematics analysis with the Faculty of Kinesiology and with the School of Dental Medicine from University of Zagreb.

## Knowledge engineering

HEARTFAID project is a EUFP6 ICT-STREP project focussed on the research and development of a knowledge enabled platform for the support of healthcare for the elderly patients suffering from heart failure syndrome (Conforti D et al., J Inform Tech Healthcare 2006: 4: 283). The Laboratory for Information Systems is leading work package 4 – Knowledge representation, discovery and management. During the first 10 months of the project we have worked on knowledge representation issues and ontology formation for the heart failure domain, based on deliverables originating from medical partners.

## Advanced measurement systems and signal processing techniques

In bio systems measurement, human mandible kinematics' parameters measurement and data acquisition is carried out using 3-D accelerometer sensors together with photogrammetric equipment. Methods for synchronization of multimedia data are developed together with extraction of kinematical parameters using adaptive integration and filtering.

Research and development of short time interval measurement methods have been continued with application to timing characterization of single-photon avalanche diodes (SPADs) and associated active quenching circuits. Measurements have been performed on stand alone devices and by virtual instrumentation (consisting of high performance DAQ cards and fast computer and data processing software LabVIEW) that control the output, process the input signals and log the data.

Research on implementation of measurement related algorithms in distributed environments is continued through the develop-

ment of the algorithm for the calculation of natural gas molar heat capacity, isentropic exponent and the Joule-Thomson coefficient. Resulting software objects are designed to fit distributed industrial measurement systems. The corresponding procedure for the automatic compensation of the compound effect of adiabatic expansion to flow measurement accuracy is developed and analyzed. A part of our recent research was also directed to multidimensional measurement data modelling based on algorithms for automatic generation of Kolmogorov-Gabor polynomials, which open the possibilities for the dimensionality reduction and the automatic modelling of multivariate measurement system functions.

## Education

1. Knowledge Discovery in Medical Domains, Dragan Gamberger, PhD Program at the Medical School, University of Zagreb.
2. Optical communication networks, Branka Medved Rogina, Graduate Program, Faculty of Electrical Engineering and Computing, Zagreb.
3. Police operational techniques, Branka Medved Rogina, Graduate Program, Police Academy, Zagreb.
4. Algorithms in Bioinformatics, Strahil Ristov, PhD Program, Faculty of Electrical Engineering and Computing, University of Zagreb.

## 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



## Research, developmental and international projects

1. HEARTFAID – A knowledge based platform of services for supporting medical-clinical management of heart failure within elderly population, Dragan Gamberger (EUFP6, ICT-STREP project)
2. Advanced Data-and Knowledge-Driven Methods for State Failure Risk Assessment, Tomislav Šmuc (NATO Security Through Science project)
3. Intelligent Data Analysis, Dragan Gamberger (Croatian-Slovenian bilateral project)
4. Inductive Databases for Genomics and Proteomics, Tomislav Šmuc (Croatian-Slovenian bilateral project)

## SELECTED PUBLICATIONS

1. Lavrač N, Gamberger D: Subgroup discovery: An experiment in functional genomics. Informatica Med Slov 2006: 11: 46.
2. Conforti D, ..., Gamberger D, Valentini M: HEARTFAID: A Knowledge Based Platform for Supporting the Clinical Management of Elderly Patients with Heart Failure. J Inform Tech Healthcare 2006: 4: 283.
3. Trontl K, Šmuc T, Pevec D: Improved SVR Model for Multi-Layer Buildup Factor Calculation. Proceedings of the 6th International Conference Nuclear Option in Countries with Small and Medium Electricity Grids 2006: S8.96.1.
4. Vojnović B: Comparison of Pulse Timing-Discriminators for Optical Distance Measurements. Proc. of ODIMAP V, 5th Topical Meeting on Optoelectronic Distance/Displacement Measurements and Applications, Spain 2006: 79: 89.





## DIVISIONAL ORGANIZATION

Head: Aleksandar Sablić

- ⇒ 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



ate education in Croatia. Last but not the least, the division members have organized 3 major international conferences including the participation of several Nobel laureates. These were: The 10<sup>th</sup> BRIJUNI CONFERENCE - Imaging in Space and Time, the 9<sup>th</sup> International Summer School on Biophysics and the 21<sup>st</sup> MATH/CHEM/COMP. Those highly regarded and well known series of conferences have generated budgets of nearly 250.000 US dollars in 2006. The majority of these contributions were from international sources (e.g. NATO, US Air Force, UNESCO, IUPAB).

## OVERVIEW OF THE DIVISION

In 2006, members of the Division published 51 contributions in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical chemistry, modelling of physical and chemical processes, structural and chemical analyses, and in biosciences. A significant part of these papers were published in the highest ranking journals in chemistry, such as *Advances in Colloid and Interface Science*, *Acta Crystallographica Section B*, the *Journal of Physical Chemistry*, the *Journal of the American Society for Mass Spectrometry*. Division members contribute extensively (43 courses) to undergraduate and gradu-

## TOP ACHIVEMENTS

### The smallest crystallized organic radical

Quinones and their reduced forms, commonly named hydroquinones, have important functions in living systems as antioxidants and redox couples for electron transfer reactions. The *p*-benzosemiquinone radical was detected in the solid state by X-ray structure analysis and EPR spectroscopy. A low-bar-

rier hydrogen bond O-H...O stabilises this radical. The two observed polymorphs of *p*-benzosemiquinone radical whose crystal structures were solved are the smallest organic radical crystallized so far (Molčanov K et al., Acta Crystallogr B 2006: B62: 1051).

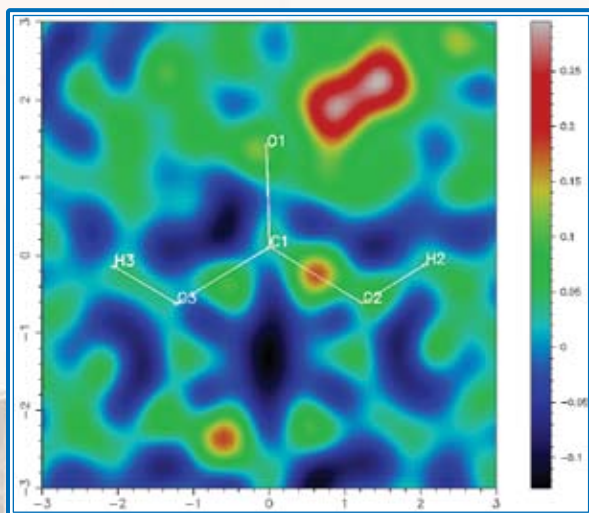


Figure 1. The difference Fourier map of *p*-benzosemiquinone radical. Red area corresponds to the delocalized hydrogen atom.

### Oxidation mechanism of aliphatic $\alpha$ -amino acids

Glycine and alanine in zwitter and anionic protonated forms were oxidized by the triplet state of anthraquinone-2,6-disulfonate

in aqueous solution. Both radicals undergo fast one step fragmentations into the same products,  $\text{CO}_2$  and  $\alpha$ -aminoalkyl radicals, but they do not constitute resonance mesomeric forms of one and the same species. This is concluded from the time-resolved Fourier transform EPR measurements and the polarization pattern analysis of the successor  $\alpha$ -aminoalkyl radicals. Results are achieved in collaboration with the Time Resolved Spectroscopy Group at the University of Leipzig, Germany (Tarabek P et al., J Phys Chem A. 2006: 110: 7293).

### Self-assembly in catanionic surfactant mixtures

Aqueous catanionic surfactant mixtures provide a great possibility to manipulate the structure of a supramolecule by variation of molar ratio and concentration of oppositely charged surfactants, as well as by combining oppositely charged surfactants of various geometries and sizes. Novel catanionic surfactants, alkylammonium cholates, crystallize into tightly packed bilayers that spontaneously form hollow cylinders (tubules) up to several micrometers in diameter. The driving forces for tubules formation are: (i) chiral packing of sodium cholate molecule in a bilayer, (ii) strong attractive interactions be-

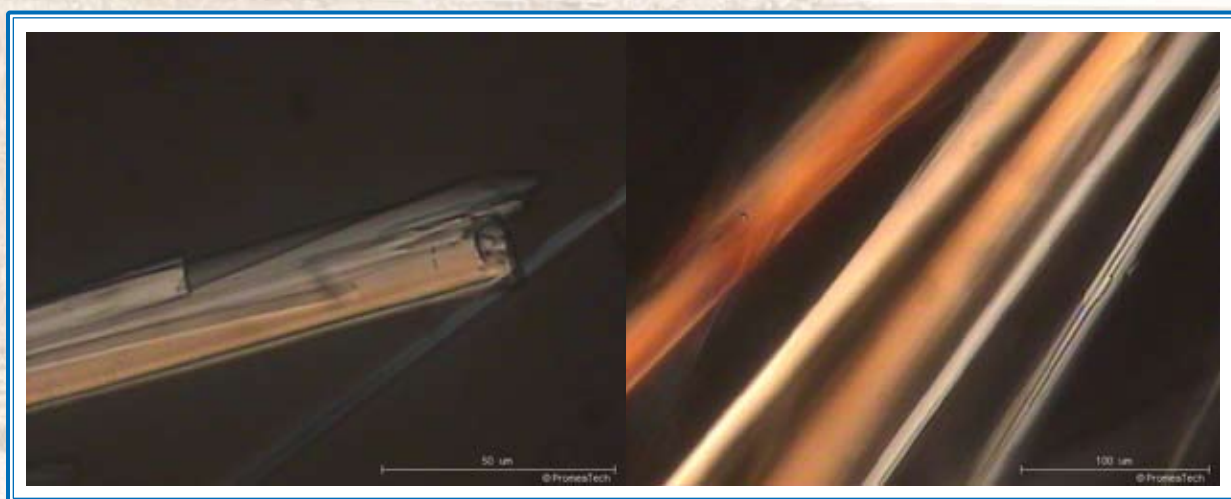


Figure 2. Representative optical micrographs of alkylammonium cholates: (a) single and (b) bundle of tubules under crossed polarizers



tween oppositely charged head groups at the bilayer/solution interface and (iii) hydrogen bonding at the bilayer surfaces (Vinceković M et al., J Disper Sci Technol 2006: 27: 1099).

### Reactive sites in flavonoids

Flavonoids are a major class of antioxidant and antiradical agents in nature and their benefits in human health promotion and disease prevention are increasingly recognized. Knowledge of their chemistry and biochemistry is far from complete and standardized chemical and biochemical methods for measuring their antioxidant activity are still lacking. The reactive site responsible for antioxidant activity of flavonoids (FI) in solution – a hydroxyl group of the B-ring – is not the site of metal ion ( $M^+$ ) attack in the gas phase. Both, mass spectra and DFT calculations of FI- $M^+$  complexes show preference for metal complexes with the carbonyl group at position 4; e.g. for  $Cu^+$  such complexes are more stable by 14-30 kcal/mol (Kazazić SP et al., J Agric Food Chem 2006: 54: 8391).

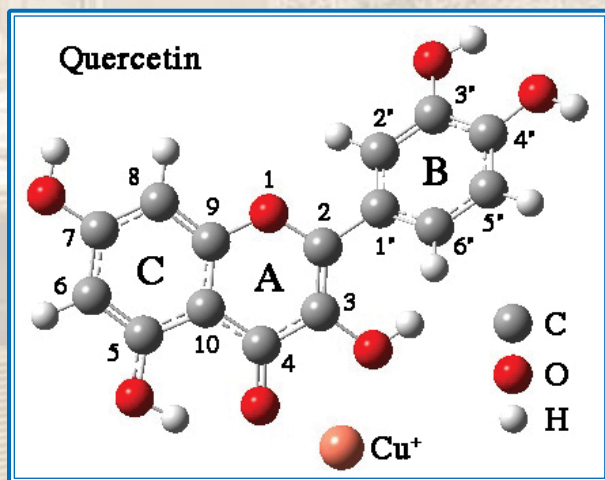


Figure 3: Structure of copper ion ( $Cu^+$ ) complex with flavonoid Quercetin

### International summer school on biophysics

The 9<sup>th</sup> International Summer School on Biophysics: Supramolecular structure and function was held in Rovinj, 16-28. September 2006. Director of the School is Greta Pifat-Mrzljak. Along with the importance of permanent education of young scientists from all around the world in the field of biosciences via interdisciplinary approaches offered by international experts, the School is recognized and accepted as a part of curriculum of distinguished European universities (e.g. University of Leeds, UK, University of Osnabrueck, Germany, University of Lisbon, Portugal, University of Maribor, Slovenia, Universities of Zagreb and Rijeka, Croatia).

### EDUCATIONAL ACTIVITIES

The division provides annually 18 undergraduate and 25 graduate courses at Universities in Zagreb, Split, Rijeka, Osijek and Maribor (Slovenia).

### AWARDS

Ante Graovac, Award of the City of Split for Scientific Achievements

### PROJECTS

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

1. Properties and behavior of atmospheric microconstituents, Tomislav Cvitaš
2. Surfactants, processes in solution and at interfaces, Nada Filipović-Vinceković
3. Reactivity and reaction mechanism, Leo Klasinc
4. Investigation on chemical reactivity and ultra-fast processes, Aleksandar Sabljic

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 lipoprotein 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 behavior of quantum systems in interaction, Tomislav Živković
15. Custom DNA synthesis, Ivan Habuš

### **Selected bilateral projects**

1. Chemical Applications of Advanced ESR-techniques, B. Rakvin (Bilateral project with Austria)
2. Structure and dynamics of biomolecules, M. Luić (Bilateral project with Slovenia)
3. Interactions of liposomes with aminoacids and peptides for targeted incorporation into organism studied by Electron Spin Resonance, V. Noethig-Laslo (Bilateral project with Slovenia)
4. Computational study of proteins structure and dynamics, S. Tomić, (Bilateral project with Slovenia)
5. Microbial lipases - search for new biocatalysts, A. Višnjevac (Bilateral project with Slovenia)
6. Electronic structure of halogenated diphenylmethanones and diphenylethanones, B. Kovač (Bilateral project with Slovenia)
7. Cyclopalladated complexes of azobenzenes, M. Čurić (Bilateral project with Slovenia)
8. Research of new materials based on carbon, A. Graovac (Bilateral project with Slovenia)

### **Selected collaborations**

1. "Investigations of calcium phosphate based biomaterials", FP6 Specific Support Action "Creating international cooperation teams of excellence in the field of emerging biomaterial surface research", Maja Dutour Sikirić
2. COST chemistry D-27 action "Origin of Life and Early Evolution", Vesna Noethig-Laslo
3. COST chemistry D-22 action "Protein-Lipid Interactions", Greta Pifat-Mrzljak
4. COST physics P-15 action "Advanced Paramagnetic Resonance Methods in Molecular Biophysics", Boris Rakvin

### **SELECTED INVITED LECTURES**

1. Bosanac SD: Physics of resonances and quantum gas. Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Observatory, Cambridge, MA, USA, 16 February 2006.
2. Dutour Sikirić M: Statistics in physical chemistry. ISM Symposium Packing and Random Packing, Tokyo, Japan, 1-3 March 2006.
3. Bonifačić M, Tarábek P, Beckert D: Oxidation mechanism of aliphatic  $\alpha$ -amino acids in aqueous solutions; electron transfer from amino vs. carboxylate functional group, 20<sup>th</sup> International Symposium on Radical Ion Reactivity (ISRIR 2006), Rome, Italy, 02-06 June 2006.
4. Graovac A: On two rather different applications of directed graphs to chemistry. Workshop on Ranking Methods and Multicriterial Decision Analysis in Environmental Sciences, Verbania, Italy, 2-3 October 2006.

### **SELECTED ORGANIZED CONFERENCES**

1. 21<sup>st</sup> MATH/CHEM/COMP, Dubrovnik, 19-24 June 2006.
2. 10<sup>th</sup> BRIJUNI CONFERENCE - Imaging in Space and Time, Brijuni, 28 August – 1. September 2006
3. 9<sup>th</sup> International Summer School on Biophysics - Supramolecular structure and function, Rovinj, 16-28. September 2006.



## SELECTED PUBLICATIONS

### Review articles

Dutour Sikirić M, Füredi-Milhofer H: The influence of surface active molecules on the crystallization of biominerals in solution. *Adv Colloid Interf Sci* 2006: 128-130: 135.

### Additional publications

1. Molčanov K, Kojić-Prodić B, Roboz M: Structural characterization of p-benzosemiquinone radical in a solid state: the radical stabilization by a low-barrier hydrogen bond. *Acta Crystallogr B* 2006: B62: 1051.
2. Došlić N: Generalization of the Rabi population inversion dynamics in the sub-one-cycle pulse limit. *Phys Rev A* 2006: 74: 013402-1.
3. Ljubić I, Sablić A: Theoretical study of structure, vibrational frequencies, and electronic spectra of polychlorinated dibenzo-p-dioxins. *J Phys Chem A* 2006: 110: 4524.
4. Kazazić SP, Butković V, Srzić D, Klasinc L: Gas phase ligation of Fe<sup>+</sup> and Cu<sup>+</sup> ions with some flavonoids. *J Agric Food Chem* 2006: 54: 8391.
5. Tarabek P, Bonifačić M, Beckert D: Time-resolved FT EPR and optical spectroscopy study on photooxidation of aliphatic  $\alpha$ -amino acids in aqueous solutions: electron transfer

from amino vs. carboxylate functional group. *J Phys Chem A* 2006: 110: 7293.

6. Novak I, Kovač B: Photochemistry via photoelectron spectroscopy: N-substituted phthalimides. *J Phys Chem A* 2006: 110: 7772.
7. Rožman M, Bertoša B, Klasinc L, Srzić D: Gas phase H/D exchange of sodiated amino acids: why do we see zwitterions? *J Am Soc Mass Spectrom* 2006: 17: 29.
8. Kveder M, Andreis M, Makarević J, Jokić M, Rakvin B: EPR study of low molecular weight organogels by means of a nitroxide spin probe. *Chem Phys Lett* 2006: 420: 443.
9. Kveder M, Merunka D, Ilakovac A, Makarević J, Jokić M, Rakvin B: Direct evidence for the glass-crystalline transformation in solid ethanol by means of a nitroxide spin probe. *Chem Phys Lett* 2006: 419: 91.
10. Sedlar J, Anđelić I, Gutman I, Vukičević D, Graovac A: Vindicating the Pauling bond-order concept. *Chem Phys Lett* 2006: 427: 418.

### Chapters in books

1. Noethig-Laslo V, Šentjerc M: Transmembrane polarity profile of lipid membranes. In: *Advances in Planar Bilayers and Liposomes - Volume 5*, A. Leitmannova Liu (Ed.). Elsevier Amsterdam, 2006. pp 367-418.





# Division of Organic Chemistry and Biochemistry

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

ZOKB

## DIVISIONAL ORGANIZATION

Head: Mirjana Eckert-Maksić

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



be emphasized that this research is multifaceted, since it also covers some aspects of materials science, environmental and medicinal chemistry. Another characteristic feature of the work is a good blend of the fundamental and applied research. The main body of the results was published in 56 scientific papers, which appeared mostly in renowned scientific journals. As to the applicative side of the research, it should be mentioned that new approaches have been unveiled in the synthesis of novel liquid crystals and chiral stationary phases. Last but not least, the spin-off company of the Institute "Chirallica" was started by members of the Division.

The Division fosters intramural and extramural collaboration including Universities in Zagreb and Osijek, and a number of research centres abroad, as evidenced by a significant number of joint papers. Members of the Division have made significant contributions to higher education by providing 9 courses at undergraduate and postgraduate levels and by supervising a number of B.Sc. (7) and Ph.D. (3) thesis. They are also active in a number of national and international societies (bodies) and serve in journal editorial boards, as well as referees of the leading scientific journals.

## OVERVIEW OF THE DIVISION

The research activities in the Division of Organic Chemistry and Biochemistry during 2006 spanned a wide spectrum of subjects ranging from modern organic syntheses, over physical organic and supramolecular chemistry, as well as spectroscopic and quantum mechanical studies of organic systems, to investigations of biologically important peptides, glycopeptides and proteins. It should

## TOP ACHIEVEMENTS

### The first examples of tubular structures of polythiolactone systems

Several new cyclic thiolactones of 12-, 14-, 24- and 28-membered rings were prepared using the tin-template method. X-ray structure analysis revealed that, in the solid state, 12- and 28- membered cyclic thiolactones form tubular assemblies. These are the first tubular structures of polythiolactone systems reported (Vujasinović I et al., Tetrahedron 2006: 62: 2868).

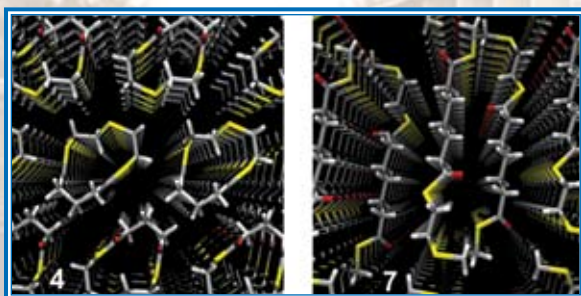


Figure 1. Examples of tubular assemblies of thiolactones

### New achievements in chemistry of gels

The discovery of a synergistic gelation effect in two-component gels is reported. An equimolar mixture of (S,S)-bis (LeuOH) oxalamide [(S,S)-1] and (S,S)-bis (leucinol) oxalamide [(S,S)-2] is able to gel up to 7 times larger volume of *p*-xylene than an equal mass of each component and up to 5 times larger a volume than an equal mass of the (S,S)-1 + (R,R)-2 or (S,S)-1 + *rac*-2 equimolar mixtures (Fig. 2). Experimental evidence showed that synergism depends on the chirality of the components, on the solvent properties and on the gel morphology (Džolić Z et al., New J Chem 2006: 30: 1411).

In addition, the preparation and the surface-enhanced Raman scattering study of the novel silver nanoparticle-hydrogel composite was reported (Miljanić S et al., Langmuir 2006: 22: 9079).

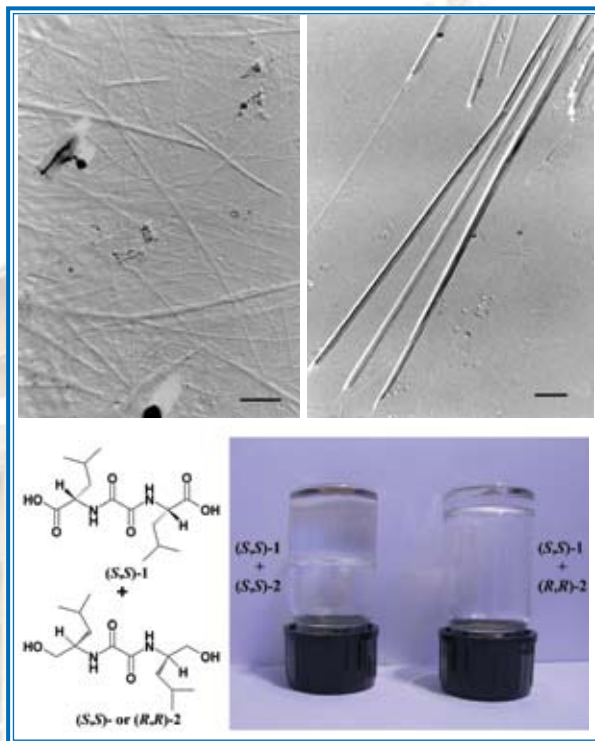


Figure 2. TEM images of Pd shadowed (a) (S,S)-1 + (S,S)-2 and (b) (S,S)-1 + (R,R)-2 *p*-xylene gels, (scale bars = 0.5 mm); (c) gels in *p*-xylene

### Towards novel liquid-crystals with flexible spacers

New series of dimeric molecules with variant flexible spacers as well as the terminal alkoxy chain length are described in which the mesogenic salicylaldimine group is linked to the alkylene spacer *via* an imino group. Mesomorphic properties of dimeric molecules revealed that the geometry, which arises from the spacer parity and the imine-spacer linkage, has an important role in the determination of the liquid-crystalline behaviour (Šepelj M et al., Chem. Mater. 2006: 18: 2050)



## Peptide-induced cytotoxicity

In collaboration with research group of Lj. Glavaš-Obrovac (Clinical Hospital Osijek, Osijek, Croatia), members of the research groups of Š. Horvat and K. Majerski reported the synthesis of a series of new peptides containing a variety of unnatural amino acids of the adamantane type, and their cytostatic activity toward malignant diseases. The peptide containing a (*R,S*)-1-adamantylglycine residue (Figure 3) was the most effective analogue especially against the most anti-tumour drug-resistant cell lines HEP-2 and SW-620. Fluorescence micrographs showed that labelled peptide can rapidly penetrate to the cellular interior of HEP-2 cells to localize mainly on the outer nuclear membrane of the tumour cells (Horvat Š et al., J Med Chem 2006: 49: 3136).

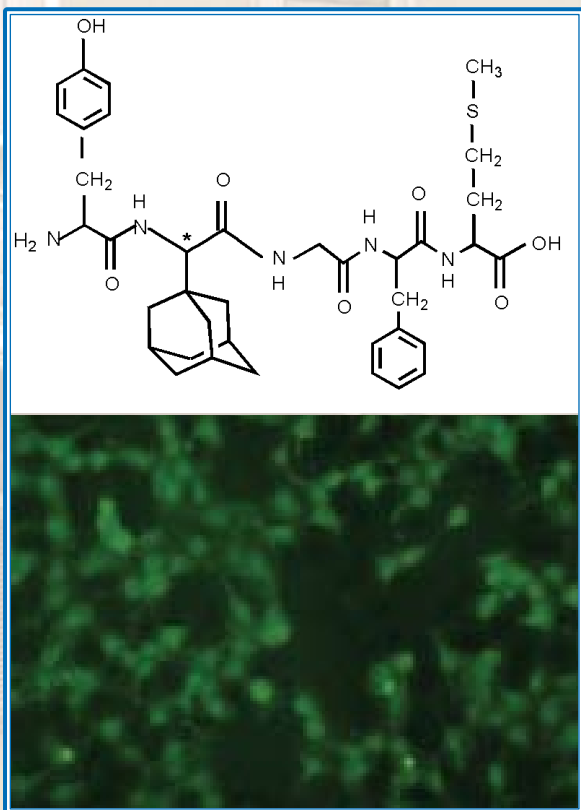


Figure 3. (a) Structure of the peptide analogue most cytotoxic against HEP-2 and SW-620 tumor cell lines. (b) Fluorescence micrograph of HEP-2 cells stained with labelled peptide

## Photochemical reactivity and photodynamics of pyrrole

Based on MR-CISD calculations, a new deactivation mechanism involving the out-of-plane ring deformation that could be responsible for more than 50% of the observed photofragments of pyrrole, was proposed. The new mechanism is shown to work complementarily to the previously proposed NH-stretching mechanism, giving therefore a more consistent and complete interpretation of pyrrole photodynamics (Barbatti M et al., J Chem Phys 2006: 125: 164323).

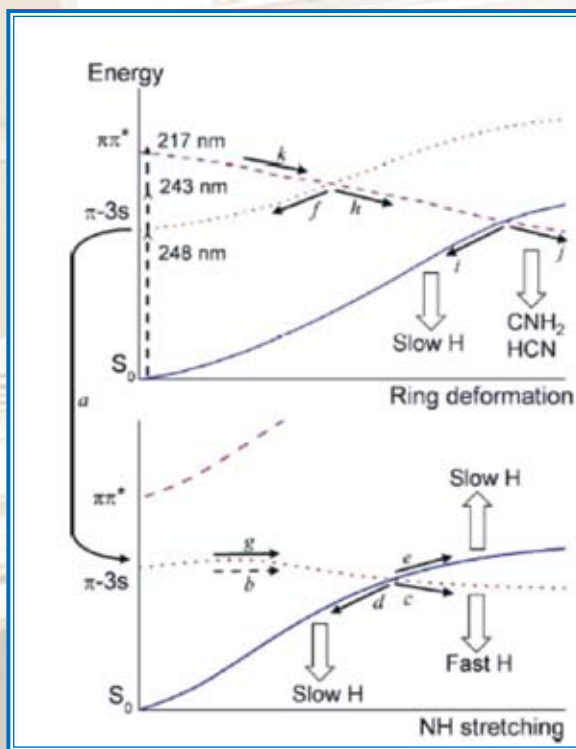


Figure 4. Qualitative scheme of the deactivation paths of pyrrole

The photochemistry of some novel pyrrole derivatives has been also the subject of experimental studies in the Division. Specifically, it was found that the excited states of stilbenopyrroles deactivate by two photochemical processes: cis-trans isomerization and hydrogen transfer of NH to the stilbene double bond (Basarić N et al., J Org Chem 2006: 71: 9382).

## Computational studies of basicity, hydride affinity and the aromaticity riddle

It was shown that phosphorus atom can be a very basic centre in some compounds. Specifically, tris- (hexamethyltri-amino-phosphazeny) phosphine has a proton affinity of 295.5 kcal mol<sup>-1</sup> and a record pK<sub>a</sub>(MeCN) value of 50 ± 1 units (Kovačević B et al., Chem Commun 2006: 1524). A meticulous analysis of hydride affinities of substituted alkynes has been performed and the results were interpreted by the original triadic formula (Vianello R et al. J Phys Chem A 2006: 110: 12870). Aromaticity, a very important notion of organic chemistry, cannot be exactly defined, which leads to many misconceptions. It is unequivocally demonstrated that Clar's aromaticity rule, which describes properties of polybenzenoid compounds, is a consequence of the σ-framework – in contrast to a widely accepted opinion that it arises due to the π-electrons (Maksic Z et al., J Phys Chem A 2006: 110: 10135).

## Theoretical Design of Strategies to Observe Elusive Reactive Intermediates in Enzyme Catalysis

The reactions catalyzed by lysine 2,3-aminomutase (2,3-LAM) and lysine 5,6-aminomutase (5,6-LAM) are thought to proceed via a mechanism involving several highly reactive free-radical species. While direct and indirect evidence have been found to support the involvement of a substrate-derived radical (S•) and a product-derived radical (P•) in these reactions, the cyclic radical intermediate (I•) remains only hypothetical. Using high-level ab initio calculations, strategies for modifying the vitamin B<sub>6</sub> cofactor (PLP) were presented that will potentially result in the first observation of the aziridinyldicarbonyl radical intermediate (I•) in the aminomutase-catalyzed reactions. (Sandala G et al. J Am Chem Soc 2006: 128: 16004).

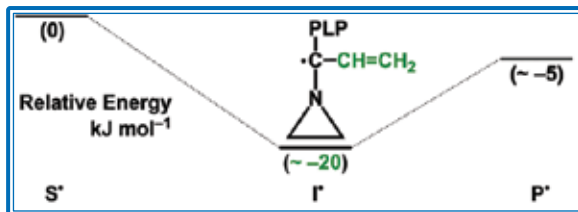


Figure 5. Potential strategy for observing the elusive cyclic intermediate in the aminomutase-catalyzed reactions

## New equipment

The infrastructure of the Division was improved by acquisition of a new CD spectrophotometer Jasco J 815, which was financially supported by the Ministry of Science, Education and Sports. This is the only CD spectrophotometer available in the Croatian academic community and it is expected to significantly improve the quality of research of optically active compounds.



Figure 6. CD spectrophotometer Jasco J 8

## AWARDS

1. Maja Šepelj - The Society of University Teachers, Scholars and other Scientists – Zagreb: Annual Reward to Young Scientists and Artists
2. Robert Vianello - National science award in 2006 - Annual award for junior researchers in the field of natural sciences



## PROJECTS

### 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  $\pi$ -Systems and Molecular Spectroscopies, Goran Baranović
9. Proton Affinity and Proton Transfer Reactions in Chemistry, Zvonimir Maksić
10. Germanium, Silicon and Tin Contained Polycyclic Structures, Davor Margetić
11. Computational Studies of Protein Structure and Function, David Smith
6. Structure-function studies on metalloproteases involved in metabolism of biologically active peptides, Bilateral Croatia-Austria project, Marija Abramić
7. Intrinsic reactivity of new molecular materials, COSTD 26 Action, WG 0014/03, Mirjana Eckert-Maksić and Zvonimir Maksić
8. Organising non-covalent chemical systems with selected functions, COST D31, WG 20, Mladen Žinić and Ivo Piantanida
9. Transcription of bioinspired and designed functional modules into nanostructured smart Gels, COST D31, WG 20, Mladen Žinić
10. Thermally processed foods: possible health implication, COST 927, WG1 and WG5, Štefica Horvat and Andreja Jakas

### Projects with industry

1. Stereoselective synthesis 3-alkyl aminoglutaric acids, PLIVA d.o.o., Zagreb, Zdenko Hameršak Design and synthesis of steroids and steroid-like derivatives, TECNA s.r.l. Area di Ricerca, Padriciano, Trieste, Italy, Kata Majerski
2. Synthesis of fluorescently-labeled macrolide probes, GlaxoSmithKline Research Institute, Zagreb, Kata Majerski
3. New biologically acceptable pH-dependent hydrogelators, Pliva, Zagreb, Mladen Žinić
4. Anthraquinone-based fluorescent organogelators, HAZU, Zoran Džolić

### Other projects

1. Pores and channels by assembly of cyclic peptides: design, molecular modelling and synthesis, Bilateral Croatian-Indian project, Kata Majerski
2. Theoretical study of bioactive molecules with property of releasing nitrogen monoxide (NO): N-nitrosohydroxylamine and its N- and O- alkyl derivatives, Bilateral Croatia-Slovenia project, Mirjana Eckert-Maksić
3. Experimental and computational study of protonated organic molecules, Bilateral Croatia-Germany project, Mirjana Eckert-Maksić
4. Modelling of organic and bioorganic compounds and processes in ground and excited states, Bilateral Croatia-Austria project, Mirjana Eckert-Maksić
5. Theoretical and experimental investigations of intramolecular and intramolecular hydrogen, Bilateral Croatia-Slovenia project, Zvonimir Maksić

### SELECTED INVITED TALKS

1. Majerski K: Thiamacrocyclic lactones with lipophilic subunits: Ag(I) selective ionophores, Workshop Symposium: Bilateral collaboration in Molecular Design and Synthesis", Leuven, Belgium, May 10-15, 2006.
2. Maksić Z B: Design of neutral organic superacids and superbases ex machina, XVIII International conference on physical organic chemistry, Warsaw, Poland, August 20-25, 2006.
3. Basarić N: Photochemistry of pyrroles: synthesis and applications in analytical chemistry, Meeting dedicated to Vladimir Prelog, Zagreb, Croatia, October 12-13, 2006.

4. Eckert-Maksić M: Guanidines – from theory to applications, Meeting dedicated to Vladimir Prelog, Zagreb, Croatia, October 12-13, 2006.
5. Horvat Š: Synthetic glycoconjugates: Models for studying interactions in biomolecular recognition and sugar-induced modifications of peptides/proteins, Meeting dedicated to Vladimir Prelog, Zagreb, Croatia, October 12-13, 2006.
6. Majerski K: Adamantane, building block in the construction of macrocyclic systems, Meeting dedicated to Vladimir Prelog, Zagreb, Croatia, October 12-13, 2006.
7. Smith DM: Specific interactions between sense and complementary peptides: what can molecular dynamics tell us?, DU NMR 2006, Mali Ston, Croatia, November 2-5, 2006.
8. Žinić B: Synthesis and biological activity of nucleobase and nucleoside derivatives, 367<sup>th</sup> Lecture for Croatian society of biochemistry and molecular biology, Croatian Society of Chemical Engineers, Rijeka, Croatia, December 07, 2006.

## SELECTED ORGANIZED CONFERENCES

3<sup>rd</sup> Meeting of the COST working group D26/0014/03, Zagreb April 28-29, 2006, principal organizer M. Eckert-Maksić

## SELECTED PUBLICATIONS

1. Sandala GM, Smith DM, Coote ML, Golding BT, Radom L. Insights into the hydrogen-abstraction reactions of diol dehydratase: relevance to the catalytic mechanism and suicide inactivation. *J Am Chem Soc* 2006; 128: 3433.
2. Horvat Š, Mlinarić-Majerski K, Glavaš-Obrovac Lj, Jakas A, Veljković J, Marczi S, Kragol G, Roščić M, Matković M, Milostić-Srb A. Tumor-cell targeted methionine-enkephalin analogues containing unnatural amino acids: design, synthesis and in vitro antitumor activity. *J Med Chem* 2006; 49: 3136.
3. Kovačević B, Maksić ZB. High basicity of phosphorus – proton affinity of tris-(tetra-

methylguanidiny)l–phosphine and tris-(hexamethyltriaminophospha-zenyl)–phosphine by the DFT calculations. *Chem Commun* 2006; 14: 1524.

4. Basarić, N, Wan, P, Competing excited state intramolecular proton transfer (ESIPT) pathways from phenol to anthracene moieties. *J Org Chem* 2006; 71: 2677.
5. Margetić D, Murata Y, Komatsu K, Eckert-Maksić M. Synthesis, X-ray and DFT study of the double bond pyramidalization in 1,7,8,9-tetraphenyl-4,10,10-trimethyl-4-aza-10-silatricyclo 5.2.1.0.2,6 decy-8-ene-3,5-dione and its germanium analogue. *Organometallics* 2006; 25: 111.
6. Miljanić S, Frkanec L, Biljan T, Meić Z, Žinić M. Surface-enhanced raman scattering on molecular self-assembly in nanoparticle-hydrogel composite. *Langmuir* 2006; 22: 9079.
7. Eckert-Maksić M, Vazdar M, Barbatti M, Lischka H, Maksić ZB. Automerization reaction of cyclobutadiene and its barrier height – an ab initio benchmark multireference average-quadratic coupled cluster study. *J Chem Phys* 2006; 125: 6.
8. Barbatti M, Vazdar M, Aquino J, Eckert-Maksić M, Lischka H. The nonadiabatic deactivation paths of pyrrole. *J Chem Phys* 2006; 125: 164323.
9. Vitale Lj, Vukelić B, Križaj I. Extracellular metalloendopeptidase of *Streptomyces rimosus*. *Arch Microbiol* 2006; 185: 183.
10. Vujasinović I, Veljković J, Mlinarić-Majerski K, Molčanov K, Kojić-Prodić B. Solid-state tubular assemblies of thiolactones: synthesis and structural characterization. *Tetrahedron* 2006; 62: 2868.
11. Džolić Z, Wolsperger K, Žinić M. Synergic effect in gelation by two-component mixture of chiral gelators. *New J Chem*. 2006; 30: 1411.

## Books and Book Chapters

1. Majerski K, Bregovec I. Nomenclature of polycyclic compounds, phane systems and spiro-compounds, Zagreb: HDKI Kemija u industriji, 2006.
2. Sandala, GM, Smith DM, Radom L. Suicide inactivation in the coenzyme B<sub>12</sub>-dependent enzyme diol dehydratase. In: Modelling structure and reactivity; Naidoo K. (editor). London: Royal Society, 2006.

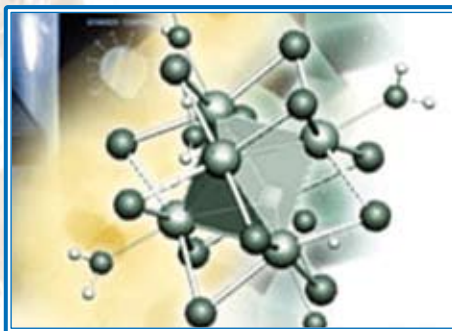


## DIVISIONAL ORGANISATION

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, Damir Kralj
- ⇒ Laboratory for radiation chemistry and dosimetry, Dušan Ražem
- ⇒ Laboratory for solid state chemistry, Želimir Blažina
- ⇒ Laboratory for complex compounds chemistry, Pavica Planinić
- ⇒ Group for ichthyopathology – biological materials, Rozelindra Čož-Rakovac



diations and their applications. The low-dose and high dose chemical dosimetry systems were developed and internationally accepted. The secondary standard dosimetry laboratory was recently established. The group for Ichthyopathology -biological materials evaluates standard values of haematological and biochemical parameters for fish species in Croatia and their alterations regarding biotic and abiotic factors. Diagnostic ichthyology services, disease prevention and therapy for marine and freshwater fishes are provided by this Group. The Division also participated in numerous cooperative activities with different industries, hospitals and different faculties at the University of Zagreb.

## OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is strongly focused on the synthesis of various materials and the investigation of their chemical, microstructural and physical properties. We are mainly investigating magnetic and nonmagnetic metal oxides, oxide glasses, glass-ceramics, zeolites, cluster compounds, organic polymers, intermetallic compounds and metal hydrides. 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 effect of ionizing ra-

## TOP ACHIEVEMENTS

### Host-guest chemistry of zeolites

The interactions of zeolite A saturated with incorporated iodine vapour was studied by vibrational spectroscopy (FT Raman and FTIR), DTG and XRD. Results show that about 50 % of iodine exists in the framework voids of zeolite A in the form of elemental iodine (molecules, clusters, crystals) and the rest exists in the ionic forms. The ionic forms of iodine (formed by disproportionation of iodine) interact with the negatively charged

aluminosilicate framework of zeolite A and with compensating sodium ions. The possible characters of interactions are discussed (Bronić J et al., Acta Chimica Slovenica 2006: 53: 166).

### Struvite to newberyite transformation

In the treatment of waste waters, particular consideration should be given to the removal of nitrogen and phosphorus. A combination of these two elements with magnesium may result in the formation of  $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$  (struvite), which has a number of potential applications. Systematic investigations of the phase transformation struvite to newberyite ( $\text{MgHPO}_4 \cdot 3\text{H}_2\text{O}$ ) extended our knowledge about the conditions under which these two compounds precipitate and about the mechanism of the conversion process (Babić-Ivančić V et al., Water Res 2006: 40: 3447).

### Structural and microstructural changes in monoclinic $\text{ZrO}_2$

High-energy ball-milling of  $m\text{-ZrO}_2$  was performed in air using the planetary ball-mill with a stainless steel milling assembly. Structural and microstructural changes during the ball-milling were monitored using XRD, Raman and Mössbauer spectroscopies, FE SEM and energy dispersive X-ray spectrometry. A very small amount of  $t\text{-ZrO}_2$  phase was found in the early stage of ball-milling and after 20 h of ball-milling a complete transformation to  $t\text{-ZrO}_2$  occurred. The combined results of precise lattice parameter measurements, FE SEM/EDS and Mössbauer spectroscopy indicated that the stabilization of  $t$ - and  $c\text{-ZrO}_2$  polymorphs at RT can be attributed to the incorporation of stabilizing aliovalent cations ( $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$  and  $\text{Cr}^{3+}$ ) introduced into the sample due to the wear and oxidation of the milling media (hardened chromium steel), (Štefanić G et al., Mater Res Bull 2006: 41: 764).

### Radiation chemistry and dosimetry

The influence of medium on the kinetics of oxidation of iron (II) ion with *tert*-butyl hydroperoxide was studied in an effort to optimize the conditions for the study of the kinetics of free radical reactions in non-polar media (Mihaljević B and Ražem D, Chem Papers 2006: 60: 253). Comparative studies of radiation-induced thermoluminescence signals from some newly developed TL detectors based on lithium fluoride, lithium borate and

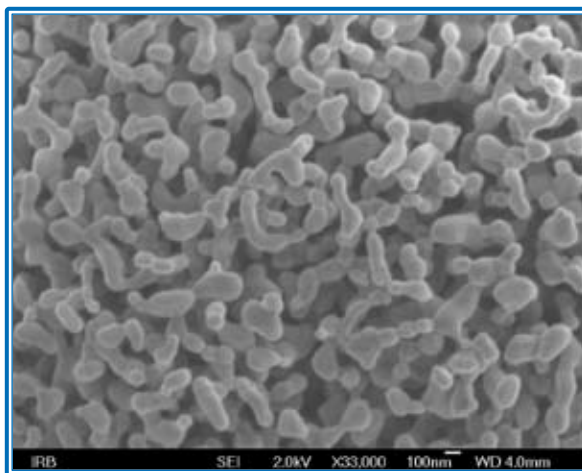


Figure 1. Microporous hematite obtained by thermal treatment of iron(III)-iodate

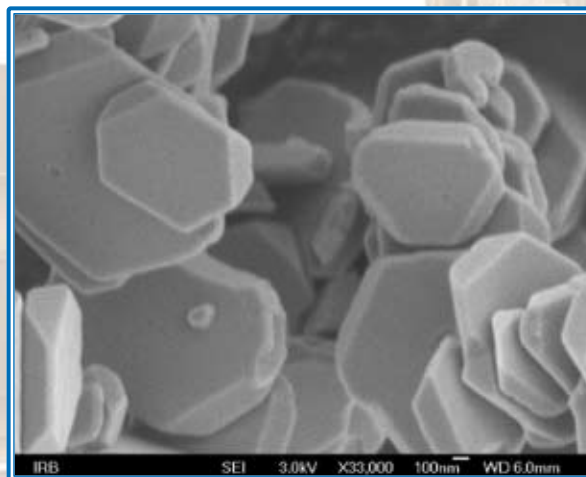


Figure 2. Tabular hematite obtained by crystallization from ferrihydrite gel



calcium fluoride were made to characterize these materials with respect to dopant elements and dosimetric performance in medical and environmental applications (Miljanić S et al., Radiat Prot Dosim 2006: 119: 191).

### Application of PIXE in polymer analysis

A fast and non-destructive method of polymer analysis was developed based on proton induced X-ray emission (PIXE) measurements. The vapour-phase corrosion inhibitor (VCI) was identified as molybdenum based. This result could not have been obtained by conventional methods of analysis. Application of PIXE in polymer analysis gave us a strong tool in the investigation of polymer ageing (Pucić I et al., Monats Chemie 2006: 137: 953).

### New alloys for hydrogen storage

New hydrogen storage alloys of the composition  $\text{LaNi}_{4.9}\text{In}_{0.1}$ ,  $\text{LaNi}_{4.8}\text{In}_{0.2}$ ,  $\text{LaNi}_{4.8}$ ,  $\text{NdNi}_{4.9}\text{In}_{0.1}$ ,  $\text{NdNi}_{4.8}\text{In}_{0.2}$  and  $\text{LaNi}_{4.8}$  were prepared, and their interaction with hydrogen was studied. All these alloys crystallize with the same hexagonal structure of the  $\text{CaCu}_5$  type (space group  $P6/mmm$ ) as do their prototypes  $\text{LaNi}_5$  and  $\text{NdNi}_5$ . Addition of indium and nickel into the alloy strongly influences the hydrogen capacity. The thermodynamic parameters of hydride formation, i.e., the entropy change, the enthalpy and the Gibbs free energy of formation have also been extracted for all alloy-hydrogen systems. From the thermodynamic point of view and high hydrogen content the  $\text{LaNi}_{4.9}\text{In}_{0.1}$  and  $\text{LaNi}_{4.8}$  alloys could be regarded as potential material for practical usage as hydrogen storage alloys (Drašner A and Blažina Ž, J Alloys Comp 2006: 420: 213).

### A New Heterotrinnuclear $[\text{Cu}^{\text{II}}\text{Cr}^{\text{III}}\text{Cu}^{\text{II}}]$ Oxalate-Bridged Compound

In designing homo- and heteropolynuclear transition metal species as the basis for potentially new magnetic materials, a very essential role, aside from the nature of the interacting metal ions, belongs to the bridging ligand that can mediate magnetic exchange interaction between two paramagnetic metal centres. Using the tris(oxalato)  $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$  complex as a building block in the reaction with copper(II) metal ions, two new heterometallic species,  $[\{\text{Cu}(\mu\text{-C}_2\text{O}_4)(\text{bpy})_2\}_2\text{Cr}(\text{C}_2\text{O}_4)]\text{NO}_3 \cdot \text{H}_2\text{O}$  and  $[\text{Cu}(\text{bpy})_3]_2[\text{Cr}(\text{C}_2\text{O}_4)_3]\text{NO}_3 \cdot 9\text{H}_2\text{O}$  ( $\text{bpy} = 2,2'$ -bipyridine) have been synthesized. Their characterization by magnetic and spectroscopic (IR, UV/VIS) means as well as the determination of their crystal structures has been accomplished. In the former one, where the central  $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$  unit acts as a bridge between two copper atoms, the ferromagnetic exchange interaction between  $\text{Cu}^{\text{II}}$  and  $\text{Cr}^{\text{III}}$  ions, with  $J = +1.20 \text{ cm}^{-1}$  (using  $H_{\text{INT}} = -J(S_{\text{Cu1}}S_{\text{Cr}} + S_{\text{Cu2}}S_{\text{Cr}})$ ) has been revealed. At the same time, this is the first crystal structure determined for an oxalate-bridged ferromagnetically coupled  $[\text{Cu}^{\text{II}}\text{Cr}^{\text{III}}\text{Cu}^{\text{II}}]$  system (Jurić M et al., Eur J Inorg Chem 2006: 2701).

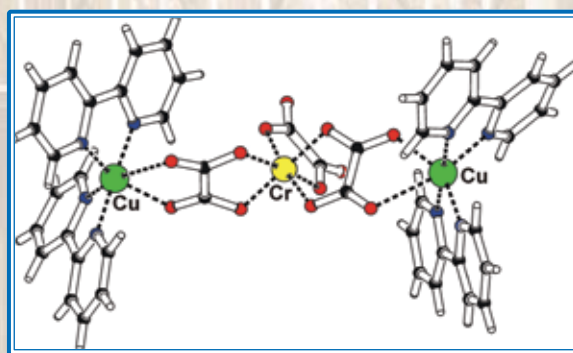


Figure 3: Copper(II) atoms bridged by the  $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$  unit in the complex cation  $[\{\text{Cu}(\mu\text{-C}_2\text{O}_4)(\text{bpy})_2\}_2\text{Cr}(\text{C}_2\text{O}_4)]^+$

## Croatian Centre for Autochthonous Species of Fish and Crustaceans Living in Carstic Waters has been established in Otočac (June 2006)

Population-genetic and phylogenetic research has been conducted through genetic mapping of autochthonous brown trout in the Gacka River. Although Gacka River is a part of the Adriatic drainage, 45 % were assigned to Atlantic haplotype Ad1 and 55 % were assigned to Danubian haplotype Da2. The presence of Atlantic and Danubian haplotypes primarily reflects introgression stemming from the stocking of hatchery-reared fish, although natural status could not be excluded. These results are of great importance for future adequate management and conservation of natural brown trout populations in the Gacka River region. (Topić Popović N et al., Fish Physiol Biochem 2006: 32: 99).



Figure 4. DNA isolation from fish tissues

## AWARDS

Svetozar Musić: Award of Croatian Academy of Science and Arts

Maria Ranogajec-Komor: Honorary Needle of the Österreichischer Verband für Strahlenschutz (for long-standing contributions to the international radiation protection community).

## 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, Damir Kralj
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. Biochemical and Molecular Reaction of Fish to the Ecosystem Status, Rozelindra Čož-Rakovac
9. Development of an adaptable technological procedure for the production of precipitated calcium carbonate, Damir Kralj (HITRA TP-01/0098-30)

### International projects and collaborative projects

1. The magnetic field influence on the calcium carbonate precipitation, Damir Kralj, Croatian-Slovenian bilateral project.
2. Polymer microcomposites and nanocomposites, Ivan Šmit, Croatian-Slovenian bilateral project.
3. Nuclear Techniques for the Protection of Cultural Heritage Artefacts in the Mediterranean Region, Branka Katušin-Ražem, International Atomic Energy Agency Technical Cooperation Project RER/1/006.
4. Quality Control Methods and Procedures for Radiation Technology, Dušan Ražem, International Atomic Energy Agency Technical Co-operation Project RER/8/010.
5. The Effect of Radiation Quality on the Response of Solid State Dosimeters, Saveta Miljanić, Croatian-Hungarian bilateral project.



6. Fundamental and Applied Research of Solid State Dosimetry, Maria Ranogajec-Komor, International project of the Croatian Academy of Sciences and Arts within the Agreement on Scientific Co-operation with the Hungarian Academy of Sciences.
7. Development of Process Control Methods in Radiation Processing, Dušan Ražem, International project of the Croatian Academy of Sciences and Arts within the Agreement on Scientific Co-operation with the Hungarian Academy of Sciences.
8. Thermally induced transformations of amorphous and crystal aluminosilicate precursors, Cleo Kosanović, Croatian-Slovenian bilateral project.

### Other projects

1. Breeding and Selection of Brook Trout in Rivers Vrnjika and Dretulja, Rozelindra Čož-Rakovac (Ministry of Agriculture, Forestry and Water Management).
2. Breeding and Selection of Autochthonous Carp in Sišćani Fish Farm, Mato Hacmanjek (Ministry of Agriculture, Forestry and Water Management).
3. Revitalization of Autochthonous Brown Trout in Karstic Rivers, Rozelindra Čož-Rakovac, (Croatian Waters).
4. Model of Revitalization and Breeding of Brown Trout, Rozelindra Čož-Rakovac (Council for Research in Agronomy - VIP, Ministry of Agriculture, Forestry and Water Management).
5. Determination of Genetic Structure and Restoration of Autochthonous Population of Brown Trout within Plitvice National Park, Rozelindra Čož-Rakovac (Plitvice National Park).

### SELECTED INVITED LECTURES

1. Milković Đ, Ranogajec-Komor M, Miljanić S, Knežević Ž, Krpan K: Comparison of Different Dosimetry Systems for Dose Measurements in Diagnostic Radiology. Second East Asia Workshop on Individual Monitoring of Ionizing Radiation, Oarai, Japan, December 2-3, 2006.

2. Miljanić S: Criticality Accidents Dosimetry System Based on Chemical and Solid State Dosimeters. Second East Asia Workshop on Individual Monitoring of Ionizing Radiation. Oarai, Japan, December 2-3, 2006.
3. Ranogajec-Komor M: Some Aspects of Solid State Dosimetry in Europe. Second East Asia Workshop on Individual Monitoring of Ionizing Radiation. Oarai, Japan, December 2-3, 2006.
4. Ranogajec-Komor M: IAEA Basic Safety Standards, EURATOM Directives and Practice in Some European Countries. Fifth Annual Convention of the Japanese Society for Radiation Safety Management, Nagoya, Japan, November 27-30, 2006.
5. Ranogajec F: Science Policy in Croatia. Second East Asia Workshop on Individual Monitoring of Ionizing Radiation. Oarai, Japan, December, 2-3, 2006.

### SELECTED PUBLICATIONS

1. Bronić J, Sekovanić L, Mužić A, Biljan T, Kontrec J, Subotić B: Host-Guest Interaction of Iodine with Zeolite A. *Acta Chimica Slovenica* 2006: 53: 166.
2. Babić-Ivančić V, Kontrec J, Brečević Lj, Kral D: Kinetics of struvite to newberyite transformation in the system  $\text{MgCl}_2\text{-NH}_4\text{H}_2\text{PO}_4\text{-NaOH-H}_2\text{O}$ . *Water Res* 2006: 40: 3447.
3. Štefanić G, Musić S, Gajović A: Structural and microstructural changes in monoclinic  $\text{ZrO}_2$  during the ball-milling with stainless steel assembly. *Mater Res Bull* 2006: 41: 764.
4. Mihaljević B, Ražem D: Influence of Medium on the Kinetics of Oxidation of Iron(II) Ion with t-Butyl Hydroperoxide. *Chem Papers* 2006: 60: 253.
5. Miljanić S, Ranogajec-Komor M, Knežević Ž, Štuhec M, Prokić M: Comparative study of  $\text{LiF:Mg, Cu, Si}$  and  $\text{Li}_2\text{B}_4\text{O}_7\text{:Cu, Ag, P}$  TL detectors. *Radiat Prot Dosim* 2006: 119: 191.
6. Zorko B, Miljanić S, Vekić V, Štuhec M, Gobec S, Ranogajec-Komor M: Intercomparison of dosimetry systems based on  $\text{CaF}_2\text{:Mn}$  TL detectors. *Radiat Prot Dosim* 2006: 119: 300.

7. Pucić I, Madžar T, Jakšić M: PIXE spectroscopy for determination of volatile corrosion inhibitor concentration in anticorrosion polymer films. *Monats Chemie* 2006: 137: 953.
8. Drašner A, Blažina Ž: Interaction of hydrogen with the  $\text{LaNi}_{4.9}\text{In}_{0.1}$ ,  $\text{LaNi}_{4.8}\text{In}_{0.2}$  and  $\text{LaNi}_{4.8}$  alloys and their Nd analogues. *J Alloys Comp* 2006: 420: 213.
9. Jurić M, Planinić P, Brničević N, Milić D, Matković-Čalogović D, Pajić D, Zadro K: New Heterometallic ( $\text{Cu}^{\text{II}}$  and  $\text{Cr}^{\text{III}}$ ) Complexes – First Crystal Structure of an Oxalate-Bridged Ferromagnetically Coupled  $[\text{Cu}^{\text{II}}\text{Cr}^{\text{III}}\text{Cu}^{\text{II}}]$  System. *Eur J Inorg Chem* 2006: 2701.
10. Topić Popović N, Strunjak-Perović I, Čož-Rakovac R, Hacmanjek M, Jadan M: Comparison of five tuna plasma analytes measured on two automated blood analyzers. *Fish Physiol Biochem* 2006: 32: 99.

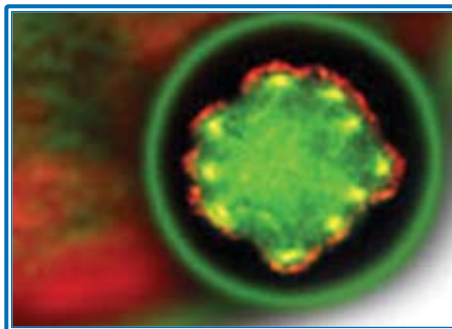


## DIVISIONAL ORGANISATION

Head: Igor Weber

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

- ⇒ Laboratory for Microbial Genetics, Krunoslav Brčić-Kostić
- ⇒ Laboratory for Molecular Microbiology, Mirjana Petranović
- ⇒ Laboratory for Molecular Genetics, Vera Gamulin
- ⇒ Laboratory for Molecular Genetics of Eukaryotes, Miroslav Plohl
- ⇒ Gene Regulation Laboratory, Mary Sopta
- ⇒ Laboratory for Experimental Cancerology, Ivica Rubelj
- ⇒ Laboratory for Genotoxic Agents, Maja Osmak
- ⇒ Laboratory for Neurochemistry and Molecular Neurobiology, Branimir Jernej
- ⇒ Laboratory for Electron Microscopy, Hrvoje Fulgosi
- ⇒ Laboratory for Chemical Biology, Volker Magnus
- ⇒ Laboratory for Biocenotic Investigations, Andrija Željko Lovrić
- ⇒ Laboratory for Cellular and Molecular Immunology, Mariastefania Antica
- ⇒ Secretary, Marija Kober



## OVERVIEW OF THE DIVISION

The research in the Division of molecular biology is based on the methods of modern molecular biology, biochemistry, cell biology, genetics, biophotonics and bioinformatics. Model organisms used in these studies include bacteria, yeast, cellular slime moulds, several invertebrates, plants and mammalian cells. The projects in our Division broadly comprise the following fields of study: 1) maintenance of genome integrity and regulation of genome variation (DNA replication, recombination and repair); 2) expression of genomic information (transcription and translation); 3) signal transduction in molecular regulation of cell division, growth, differentiation and senescence; 4) cellular responses to toxic agents and resistance to cytostatics and antibiotics; 5) regulatory mechanisms of photosynthesis; 6) dynamical processes in the cytoskeleton, and finally 7) evolution of genes and genomes. The primary purpose of these research projects is a general broadening of our knowledge of biological processes at the molecular level and the underlying principles of life, as well as the training of young scientists for professional work in the field of molecular biosciences, including biomedicine and biotechnology.

In 2006, members of the Division of Molecular Biology participated in teaching more than 30 subjects at Croatian universities. During that year they also supervised more than 20 diploma, MSc, and PhD theses. A series of practical courses in biology and medicine was organized in our Division by Andreja Ambriović Ristov (<http://www.tecajevi-irb.com>).

## TOP ACHEIVEMENTS

### Genome restoration in *Deinococcus radiodurans*

We have revealed how bacterium *Deinococcus radiodurans*, one of the most radiation resistant organisms known, restores its genome shattered by radiation. The process

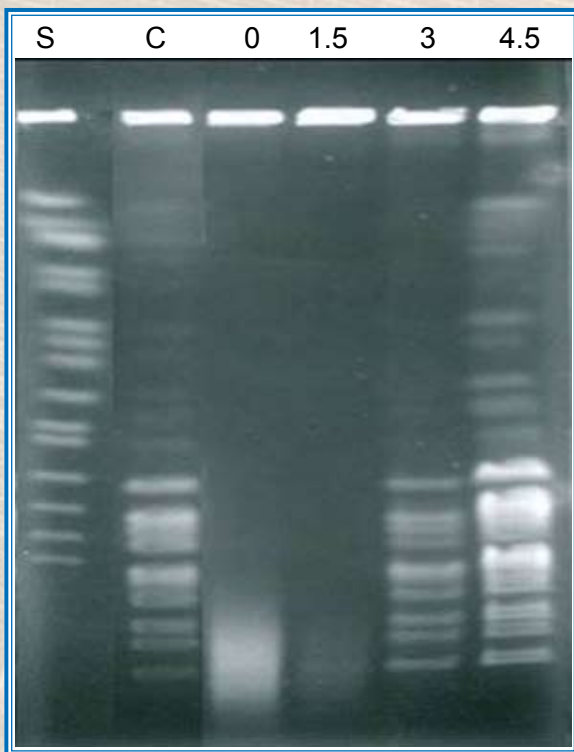


Figure 1: DNA repair after 7-kGy  $\gamma$ -irradiation of *D. radiodurans* as followed by pulsed-field gel electrophoresis. S: *S. cerevisiae* chromosomes as molecular mass standards. C: DNA from unirradiated cells. 0 – 4.5: DNA from irradiated cells at different time points (hours) during postirradiation incubation.

involves two stages: an extended synthesis-dependent strand annealing (ESDSA) followed by homologous recombination. In ESDSA, chromosomal fragments produced by radiation are used both as primers and templates for massive synthesis of long single strand extensions. The synthesized strands then anneal, thereby accurately connecting contiguous DNA fragments into linear intermediates. These intermediates are finally matured by RecA-dependent crossovers into functional circular chromosomes that are patchworks of old (synthesized before radiation) and new (synthesized after radiation) double-stranded DNA blocks (Zahradka K et al., Nature 2006: 443: 569).

### Two types of *sbcB*-sensitive RecF recombination pathways in *Escherichia coli*

*Escherichia coli* cells mutated in *recBC* genes are defective for the main RecBCD pathway of recombination and recombinational DNA repair. This defect can be compensated by suppressor mutations in *sbcB* and *sbcC(D)* genes, which activate an alternative RecF recombination pathway. We found that two *sbcB* mutations, *sbcB15* and  $\Delta$ *sbcB*, have different effects on recombination in *recBC* (*sbcC*) background and activate two types of RecF recombination pathway that differ in their enzymatic requirements (Zahradka K et al., J Bacteriol 2006: 188: 7562).

### SOS induction

The SOS response results in the coordinately induced expression of more than 40 genes which occurs when cells are treated with DNA-damaging agents. We found that RecA-loading activity is essential for SOS induction after UV-irradiation and that strain with inactivated RecA-loading activity of RecBCD enzyme exhibits constitutive expression of the SOS regulon. Surprisingly, this constitutive SOS expression is depen-



dent on the RecJ nuclease but not on RecFOR, implying that there is a different mechanism of RecA-loading for constitutive SOS expression (Ivančić-Baće I et al., J Bacteriol 2006: 188: 5024).

### UV-induced restriction alleviation

Chromosomal DNA is protected from degradation by methylation of target sequences. However, when unmethylated target sequences are generated in the bacterial chromosome, the endonuclease activity of the EcoK1 restriction-modification enzyme is inactivated by the ClpXP protease, and DNA is protected. This process is known as restriction alleviation and it can be induced by UV-irradiation. Our genetic analysis showed that UV-induced restriction alleviation is dependent on the excision repair protein UvrA, the RecA-loading activity of the RecBCD enzyme, and primosome assembly activity of the PriA helicase. (Ivančić-Baće I et al., Genetics 2006: 174: 2137).

### The role of exonucleases in recombination in *E. coli*

The RecBCD enzyme initiates the majority of homologous recombination in wild-type *E. coli*. When the enzyme lacks its RecD subunit, the resulting RecBC enzyme is devoid of nuclease activity but is still recombination proficient. To test for possible compensation of this defect, multiple exonucleases present in *E. coli* were inactivated and a complex pattern of their overlapping/competing activities was revealed. These exonucleases were shown to be essential for cell viability, DNA repair and homologous recombination, dependent on RecBC enzyme (Đermić D, Genetics 2006: 172: 2057; Đermić D et al., Genetics 2006: 173: 2399).

### Repetitive DNA sequence evolution

Reasons for long-time persistence of some satellite DNAs (tandemly repeated non-coding DNA sequences in heterochromatin) are poorly understood. Characterization of the set of related satellite DNAs coexisting in the form of a library in parthenogenetic root-knot nematode species disclosed conserved domains with three different levels of sequence variability. We conclude that sequence dynamics of these satellites is driven by interplay of selective constraints and stochastic events, probably as a consequence of functional interactions in heterochromatin (Meštrović N et al., Mol Biol Evol 2006: 23: 2316).

### Bacterial SSBs

Single stranded DNA binding proteins (SSBs) play a crucial role in DNA replication, recombination and repair. It is known that eukaryotic SSBs are regulated by phosphorylation on several serine and threonine residues. We have shown that bacterial SSBs are phosphorylated on tyrosine. This is the first evidence that an essential bacterial protein undergoes specific posttranslational modification and raises exciting possibility

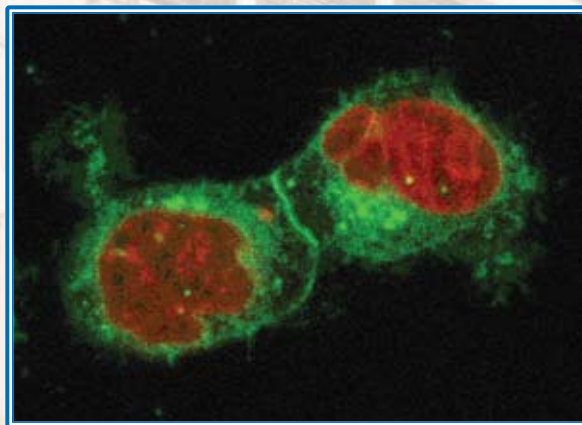


Figure 2: Dil staining of MDA-MB-231 cells. Merged image of Dil and DRAQ5 stained cells observed under confocal microscope. Dil is incorporated into cells' membranes (pseudo green), DRAQ5 is incorporated into nuclei (red).

that the post-translational regulation of SSBs in bacteria may be important for regulating DNA repair and replication (Mijaković I et al., Nucleic Acid Res 2006: 34: 1588).

### Spontaneous senescence in MDA-MB-231 cells

When a telomere, a specialized structure at the end of a chromosome, achieves a critical minimal length, the cell enters a non-dividing state known as cellular senescence. The immortal cell line MDA-MB-231 has active telomerase, which prevents telomere shortening and allows cells' permanent divisions. We investigated possible mechanisms that cause the appearance of non-growing fraction of cells in cultures of MDA-MB-231, and concluded that stress and genome instability, rather than variation in telomerase activity or telomere shortening, affect individual cells (Ćukušić A et al., Cell Proliferation 2006: 39: 205).

### Regulation of chloroplast gene expression

We characterized a novel chloroplast protein TCP34 that was not present in etioplasts but appeared only in developing chloroplasts. The *in vitro* translated precursor could be imported into intact spinach chloroplasts and showed stable association with thylakoid membranes. The high molecular weight thylakoid TCP34 variant was found in association with a transcriptionally active protein/DNA complex (TAC) from chloroplasts and recombinant TCP34 showed specific binding to chloroplast DNA (cpDNA). Based on the structural properties and biochemical analyses we propose a putative regulatory function of TCP34 in the plastid gene expression (Weber P et al., J Mol Biol 2006: 357: 535).

## MODERN FACILITIES, METHODS AND EQUIPMENT

### Centre for DNA sequencing

The DNA centre for DNA sequencing was established in 2006 as a part of the Laboratory for Molecular Genetics and under the supervision of Helena Četković. It offers a microsatellite genotyping method for external users. More than 2000 sequence analyses were already performed at the DNA centre using ABI-Prism 3100 Sequencer.



Figure 3: DNA sequencing facility.

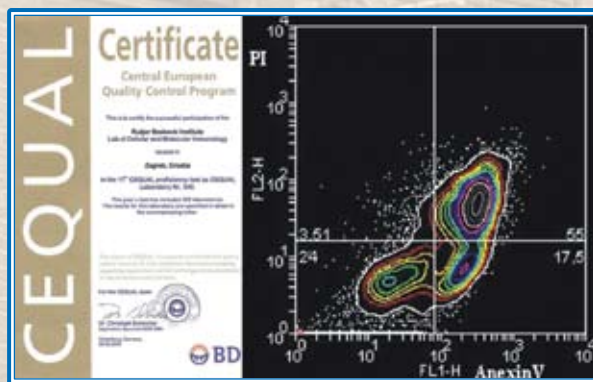


Figure 4: CEQUAL certificate to the Laboratory of Cellular and Molecular Immunology and a sample flow cytometry analysis.



## Flow cytometer

The flow cytometer uses the principles of light scattering, light excitation, and emission of fluorochrome molecules for multi-parameter cell analysis. Under the supervision of Mariastefania Antica, several research groups are studying diverse physical characteristics of cells, DNA content, cell cycle, and apoptosis markers.

## PROJECTS

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

1. The role of recombination in DNA repair and genome stability, Krunoslav Brčić-Kostić
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, Marija-Mery Sopta
7. Molecular mechanisms of immortalization 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, Branko Jernej
11. Hydrodynamics of the cerebrospinal fluid, Darko Orešković
12. Structure and function of plastids and the cytoskeleton, Hrvoje Fulgosi
13. Dynamics and genetics of bioactive molecules, Volker Magnus
14. Endemic and relict phytocenoses of Croatia and their mycoflora, Andrija Željko Lovrić
15. Transcriptional control of lymphocyte development – its role in leukemogenesis, Mariastefania Antica

## Other projects

1. Dynamics of protein recruitment into a cortical complex, Igor Weber (MZOŠ, DAAD bilateral project with Germany, 911-02/05-04/11)
2. Engineering of GDSL-hydrolases and application of *Streptomyces* expression system, Dušica Vujaklija (MZOŠ, bilateral project with Austria, 911-02/05-06/35)
3. Genetic diversity and evolutionary processes of irises along the Dinaric Alps, Hrvoje Fulgosi (MZOŠ, Cogito bilateral project with France, 910-08/04-01/0094)
4. Increased effect of anti-cancer drugs by silencing the target genes in tumor cells, Maja Osmak (MZOŠ, bilateral project with Macedonia, 910-08/06-01/00268)
5. Molecular analysis of the transcriptional regulation of Helios, an Ikaros gene family member in human leukemic cells, Mariastefania Antica (MZOŠ, bilateral project with Austria, 911-02/05-06/20)
6. Plant hormones – Physiology, biochemistry and application, Volker Magnus (MZOŠ, collaborative project, 0098903)
7. Propagation of the American highbush blueberry (*Vaccinium corymbosum* L.), Branka Salopek-Sondi (Center for agriculture at high altitudes, Primorsko-goranska county, applied collaborative project)
8. Propagation of aronia (*Aronia melanocarpa* L.), Branka Salopek-Sondi (Center for agriculture at high altitudes, Primorsko-goranska county, applied collaborative project)
9. Rho GTPases and adhesion mediated tumor cell resistance to cisplatin, Maja Osmak (MZOŠ, DAAD bilateral project with Germany, 911-02/05-04/09)
10. Synthesis and evaluation of new potential cytostatics from diazene family, Maja Osmak (MZOŠ, bilateral project with Slovenia, 910-08/05-01/00159)
11. Structural and functional analysis of noncoding heterochromatic DNA in insect *Tribolium castaneum*, Đurđica Ugarković (EC FP6 Marie Curie Transfer of Knowledge project, MTKD-CT-2006-042248)
12. Visualization and analysis of three-dimensional microscopic fluorescence distributions, Igor Weber (MZOŠ, IT application project, 2004-248)

## SELECTED INVITED LECTURES

1. Gamulin V: How complex is sponge genome? Marie Curie Summer School BIOCAPITAL. Rovinj, Croatia, August 21-26, 2006.
2. Jurić S, Lepeduš H, Hazler-Pilepić K, Jeličić B, Fulgosi H: TROL integrates chloroplast redox signalling. 4<sup>th</sup> Slovenian Symposium on Plant Biology with International Participation. Ljubljana, Slovenia, September 12-15, 2006.
3. Salopek-Sondi B, Tomašić A, Magnus V: Wheat auxin amidohydrolase: a regulator of auxin activity in plants. Third Symposium of the Croatian Society of Plant Physiologists, 9<sup>th</sup> Croatian Biological Congress. Rovinj, Croatia, September 23-29, 2006.
4. Ugarković Đ: Functional elements in satellite DNAs. International Conference on Immunogenomics and Immunomics, Budapest, Hungary, October 8-12, 2006.
5. Vujaklija D: An Introduction to GMO. EURO-TOX 2006/6 CTDC Congress. Cavtat, Croatia, September 20-24, 2006.
6. Vujaklija D: A novel substrate of bacterial tyrosine kinase. Congress of the Croatian Society of Biochemistry and Molecular Biology. Vodice, Croatia, October 3-7, 2006.
7. Weber I: Architecture and dynamics of the cell cortex. EMBO/HHMI Central European Scientists Meeting. Cavtat, Croatia, June 15-17, 2006.

## SELECTED ORGANIZED CONFERENCES


1. Ugarković Đ. EMBO/HHMI Central European Scientists Meeting 2006. Cavtat, Croatia, June 15-17, 2006.
2. Vujaklija D. Dealing with and debating about GMOs. Satellite course at the 43<sup>rd</sup> Congress of the European Societies of Toxicology. Cavtat, Croatia, September 20-24, 2006.

## SELECTED PUBLICATIONS

### Research articles

1. Baharoglu Z, Petranović M, Flores M-J, Michel B. RuvAB is essential for replication forks reversal in certain replication mutants. *EMBO J* 2006; 25: 596.
2. Đermić D. Functions of multiple exonucleases are essential for cell viability, DNA repair and homologous recombination in *recD* mutants of *Escherichia coli*. *Genetics* 2006; 172: 2057.
3. Đermić D, Zahradka D, Petranović M. Exonuclease requirements for recombination of  $\lambda$ -phage in *recD* mutants of *Escherichia coli*. *Genetics* 2006; 173: 2399.
4. Ivančić-Baće I, Vlašić I, Čogelja-Čajo G, Brčić-Kostić K, Salaj-Šmic E. Roles of PriA protein and double-strand DNA break repair functions in UV-induced restriction alleviation in *Escherichia coli*. *Genetics* 2006; 174: 2137.
5. Ivančić-Baće I, Vlašić I, Salaj-Šmic E, Brčić-Kostić K. Genetic evidence for the requirement of RecA loading activity in SOS induction after UV irradiation in *Escherichia coli*. *J Bacteriol* 2006; 188: 5024.
6. Majhen D, Gabrilovac J, Eloit M, Richardson J, Ambriović-Ristov A. Disulfide bond formation in NGR fiber-modified adenovirus is essential for retargeting to aminopeptidase N. *Biochem Biophys Res Commun* 2006; 348: 278.
7. Meštrović N, Castagnone-Sereno P, Plohl M. Interplay of selective pressure and stochastic events directs evolution of the MEL 172 satellite DNA library in root-knot nematodes. *Mol Biol Evol* 2006; 23: 2316.
8. Mijaković I, Petranović D, Maček B, Čepo T, Mann M, Davies J, Jensen PR, Vujaklija D. Bacterial single-stranded DNA-binding proteins are phosphorylated on tyrosine. *Nucleic Acids Res* 2006; 34: 1588.



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9. Pozhitkov A, Noble P, Domazet-Lošo T, Nolte A, Staehler P, Beier M, Tautz D. Tests of rRNA hybridization to microarrays suggest that hybridization characteristics of oligonucleotide probes for species discrimination cannot be predicted. *Nucleic Acids Res* 2006: 34: e66.
  10. Tarkowski P, Tarkowska D, Novák O, Mihaljević S, Magnus V, Strnad M, Salopek-Sondi B. Cytokinins in the perianth, carpels, and developing fruit of *Helleborus niger* L. *J Exp Bot* 2006: 57: 2237.
  11. Weber P, Fulgosi H, Piven I, Muller L, Krupinska K, Duong VH, Herrmann RG, Sokolenko A. TCP34, a nuclear-encoded response regulator-like TPR protein of higher plant chloroplasts. *J Mol Biol* 2006: 357: 535.
  12. Zahradka K, Slade D, Bailone A, Sommer S, Averbeck D, Petranović M, Lindner AB, Radman M. Reassembly of shattered chromosomes in *Deinococcus radiodurans*. *Nature* 2006: 443: 569.
  13. Zahradka K, Šimić S, Buljubašić M, Petranović M, Đermić D, Zahradka D. *sbcB15* and  $\Delta sbcB$  mutations activate two types of RecF recombination pathway in *Escherichia coli*. *J Bacteriol* 2006: 188: 7562.

## Invited review articles

1. Ambriović-Ristov A, Osmak M. Integrin-mediated drug resistance. *Curr Signal Transduction Ther* 2006: 1: 227 (*written upon invitation from the Editor of a new expert review journal in signal transduction therapy*).
2. Majhen D, Ambriović-Ristov A. Adenoviral vectors - How to use them in cancer gene therapy? *Virus Res* 2006: 119: 121 (*first on the list of most read articles within the journal Virus Research, counted by article downloads in ScienceDirect, July-September 2006*).
3. Petković H, Cullum J, Hranueli D, Hunter IS, Perić-Concha N, Pigac J, Thamchaipenet A, Vujaklija D, Long PF. Genetics of *Streptomyces rimosus*, the oxytetracycline producer. *Microbiol Mol Biol Rev* 2006: 70: 704.
4. Traven A, Jeličić B, Sopta M. Yeast Gal4: a transcriptional paradigm revisited. *EMBO Rep* 2006: 7: 496.
5. Weber I. Is there a pilot in a pseudopod? *Eur J Cell Biol* 2006: 85: 915.





# Division of Molecular Medicine

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



## DIVISIONAL ORGANIZATION

Head: Krešimir Pavelić

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

- ⇒ 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
- ⇒ Animal Quarters, Ranko Stojković

## OVERVIEW OF THE DIVISION

The mission of the Division of Molecular Medicine is to expand and strengthen the knowledge of the nature of diseases 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 molecular targeted therapy for use against cancer and viral diseases, new diagnostic tools and research aimed at deciphering the molecular basis of disease, and tools based on *-omics* approaches. As such, the Division is emerging as a centre of excellence, for research in molecular approaches to the study of disease.

## TOP ACHIEVEMENTS IN BASIC RESEARCH

### Nm23-H1 gene downstream targets

Nm23-H1 gene downstream targets have been identified by subjecting Nm23-H1 over-expressing CAL 27 cells (oral squamous cell carcinoma) to microarray analysis. The genes with changed expression patterns could be clustered into several groups: transforming growth factor  $\beta$  signalling pathway, cell adhesion, invasion and motility, proteasome machinery, cell-cycle, epithelial structural and related molecules.

### Novel p53 isoforms and inhibitory p53/p73 network

Novel p53 isoforms and an inhibitory p53/p73 network have been characterized. Using natural promoters with a p73/p53 binding site driving a luciferase promoter reporter assays in p-53-null cells have been performed. Delta Np53 isoforms down-regulated another tumour suppressor gene, p73, a member of the same p53 family. Inhibitory interaction led to stabilization of Tap73. The discovery of inhibitory p53/p73 network could have a major clinical impact in prognostic use and p53 targeted drug design.

### Aberrant FHIT gene in malignant thyroid cancers

The majority of the malignant thyroid cancers displayed aberrant expression of FHIT gene, concomitant with p53 gene inactivation, followed by low rate of apoptosis, and malignancy. Concomitant aberration of FHIT gene and p53 could be responsible for development of highly malignant types of thyroid cancer and may be considered as a prognostic marker for these tumours (Pavelic K et al., Mutation Res 2006: 599: 45).

### Serotonin in PTSD

Increased platelet serotonin concentration was found in veterans with combat related posttraumatic stress disorder (PTSD) complicated with psychotic symptoms, especially delusions. The data confirm the hypothesis that psychotic PTSD is biologically distinct form of PTSD, and that platelet serotonin concentration might be used as a trait marker for particular (psychotic) subtype of PTSD (Pivac N et al., J Affect Disord 2006: 93: 223).

### Opioid peptides and oxidant/antioxidant enzyme activity

The fact that the effect of opioid peptides on the both the transcriptional level and on the level of oxidant/antioxidant enzyme activity was found to be related not only to age, but also to gender, may have therapeutical implications.

### Genuine yeast model for lipid peroxidation

A yeast strain conditionally expressing the D12 desaturase gene that provides a novel and well-defined eukaryotic model in lipid peroxidation research was introduced. It revealed that production of poly-unsaturated

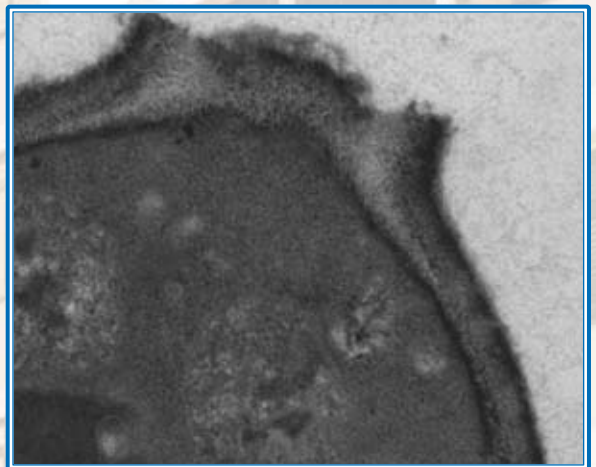


Figure1a: Normal morphology of budding yeast (electron microscope, original magnification: 56,000x)



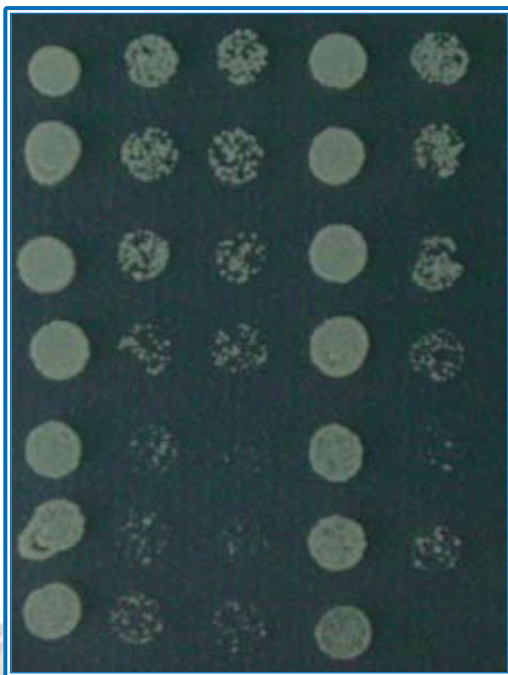


Figure 1b: Sensitivity of PUFA-producing yeast to acute stress. Strains were exposed to various stressors for 4h and afterwards plated on solid media for viability test.

fatty acids is associated with spontaneous production of 4-hydroxynonenal (HNE) that is considered as “second messenger of free radicals” and “major bioactive marker of lipid peroxidation” (Čipak A et al. Free Radical Biol Med 2006; 40: 897).

### Relevance of lipid peroxidation in colon carcinogenesis

Association of the lipid peroxidation product acrolein, which is considered as major environmental lipid peroxidation pollutant (abundant in automotive and cigarette smoke), with the transition of benign to malignant colon tumours was described for the first time. Complementary to that, c-Jun N-terminal kinase upregulation was described as a key event in the proapoptotic interaction between TGF- $\beta$ 1 and HNE in colon mucosa, while iron metabolism was indicated as important parameter of tumour progression

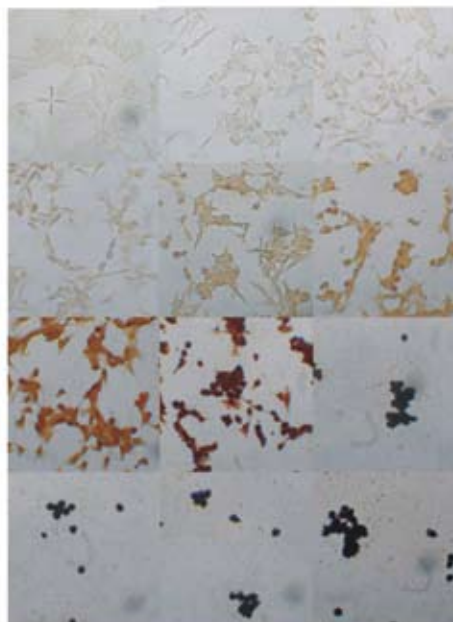
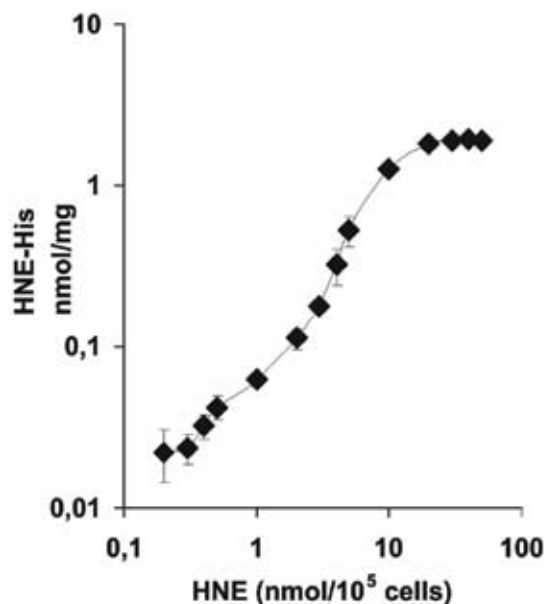


Figure 2. HNE-protein conjugates determined by immunocytochemistry and ELISA in HOS cell cultures after treatment with HNE. Concentrations of HNE used to treat cells were expressed in nmol/10<sup>5</sup> cells and indicated on photos.

and dissemination (Prutki M et al., Cancer Lett 2006: 238: 188; Biasi F et al., Free Radical Biol Med 2006: 40: 443).

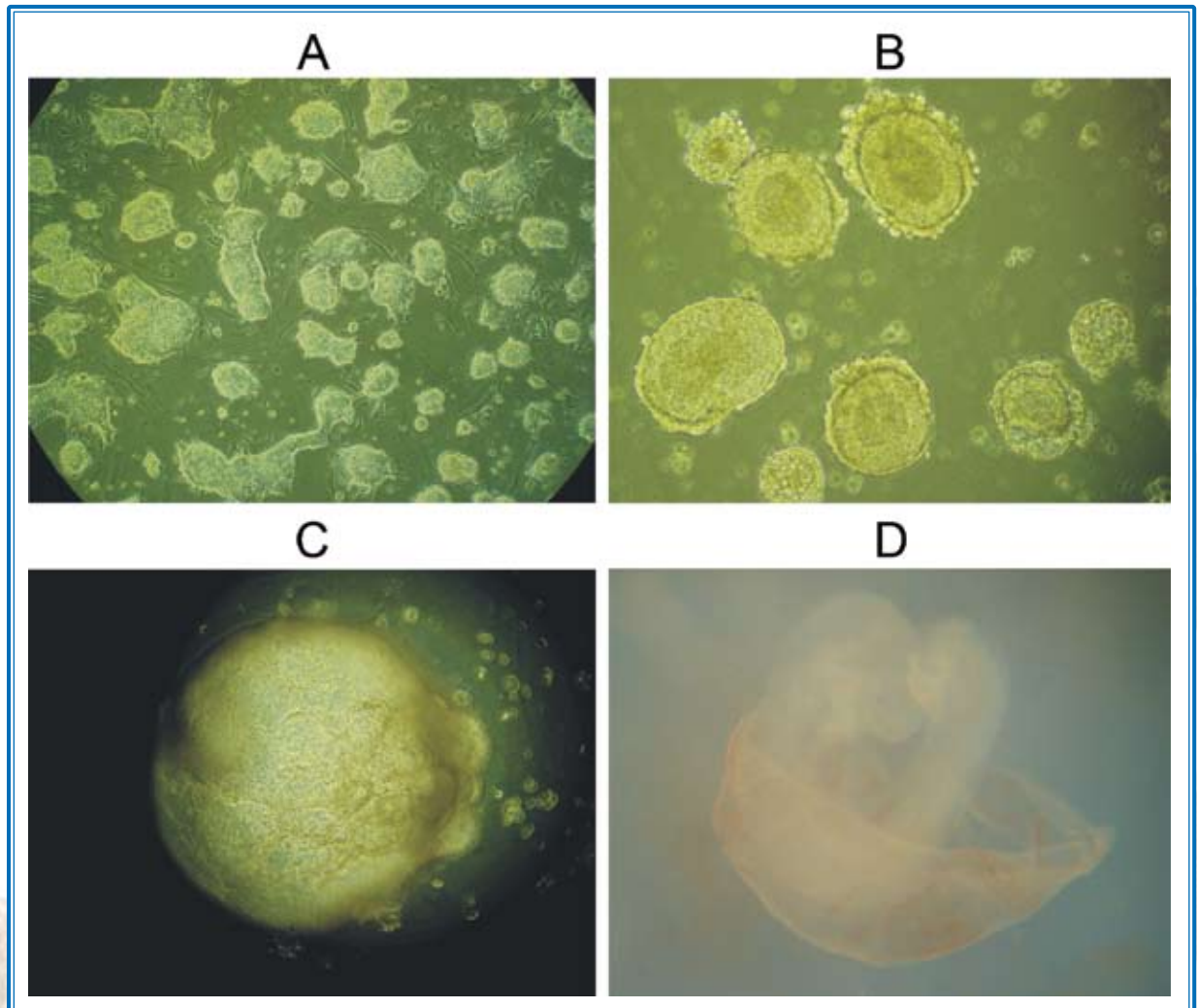
### **S-Adenosylhomocysteine hydrolase (AdoHcyase) deficiency**

S-Adenosylhomocysteine hydrolase (AdoHcyase) deficiency is a new human disorder. Investigating the molecular mechanisms responsible for the pathogenesis of the disease, we have shown that a single mutation at tyrosine 143 of human AdoHcy-

ase renders the enzyme thermosensitive and reduces its enzymatic activity to only 25% of normal (Beluzic R et al., Biochemical J 2006: 400: 245).

### **Retargeting of NGR fibre-modified adenovirus to aminopeptidase (APN)**

The peptide motif NGR (asparagine–glycine–arginine) is known to bind to aminopeptidase N. Five adenoviruses bearing NGR in the HI loop of the adenoviral fibre protein



*Figure 3. Embryonal cells. Type I Diabetes mellitus is caused by an autoimmune process which destructs beta cells of the Langerhans islets. The derivation of embryonic stem cell line from 3.5 days old embryos (blastocysts) of non-obese diabetic mouse strain enables the growth of blastocysts, essential for maintenance of stem cell pluripotency.*

*A, embryonic stem cells; B, embryoid body; C, embryoid body in tissue culture; D, mouse fetal body.*



were constructed and their targeting properties to aminopeptidase N were compared. Adenoviruses containing NGR within cyclic sequences retargeted viruses mainly to aminopeptidase N, while adenoviruses containing NGR within linear sequences, retargeted adenoviruses mainly to  $\alpha_v\beta_3$  integrin (Majhen et al., Biochem Biophys Res Com 2006: 348: 278).

## **TOP ACHIEVEMENTS IN APPLIED RESEARCH**

### **Development of the first HNE-His ELISA**

Intensive work on immunodetection of HNE led to development of the first ELISA for HNE-histidine adducts. The assay was designed to quantify development of HNE-protein adducts in cultured cells and was proven to be efficient both for cellular physiology and for pathophysiology of oxidative stress and lipid peroxidation.

### **Oxidative stress in convalescence after acute myocardial infarction**

The results of a clinical study showing persistence of systemic oxidative stress after myocardial infarction treated by percutaneous coronary intervention indicate that patients are released from hospital under oxidative stress associated with the healing of the damaged tissue and inflammatory stress response.

### **Polymorphisms and severity of tuberculosis**

Association between polymorphism in the IFN- $\gamma$  gene and development and severity of tuberculosis has been found. Particular combination of IFN- $\gamma$  and IFN- $\gamma$  receptor-1 SNP's might offer better protection against tuberculosis.

### **Polymorphisms in late total hip arthroplasty failure**

TGF- $\beta$ 1 signal sequence ( $^{29}\text{T}\rightarrow\text{C}$ ) transitions and IL-6 promoter ( $-579\text{G}\rightarrow\text{A}$ )/( $-572\text{G}\rightarrow\text{C}$ ) transitions are predictive for the time to onset of aseptic instability after late total hip arthroplasty failure.

### **A novel therapeutic indication**

Treatment-resistant depression is a common clinical problem, often complicated with suicidal ideations and greater lifetime functional impairment, and represents a considerable challenge to management and treatment. The add-on treatment with atypical antipsychotic, quetiapine, improved the clinical state in treatment resistant depressed patients. The data suggest that quetiapine is a safe and effective therapeutic strategy for patients who are resistant to previous antidepressant treatment (Šagud M et al., Psychopharmacology, 2006: 187: 511).

### **Novel hepatoprotective antioxidants**

The potential effectiveness of 1,4-dihydroisonicotinic acid derivatives in the prevention of lipid peroxidation was proven. Description of these findings was highlighted by the use of genuine murine liver stem cell cultures and analytical models that revealed potential hepatoprotective use of such compounds.

### **New preparation for diabetic neuropathy**

The synthetic zeolites (mineral) and selected herbal proteins successfully regulate glycemia and also arrest the process of apoptosis caused by pathological accumulation of  $\text{Ca}^{2+}$  ions in the cytoplasm of nerve cells. The mineral-protein preparation is applied for the prevention of the development

of diabetic neuropathies in persons suffering from diabetic's late complication (Patent US7, 074, 437 - Mineral-protein preparations (MPP) and neuropathies in diabetes).

### Screening of newly synthesized anticancer compounds

During 2006 over 160 newly synthesized compounds, such as cyano- and amidino-substituted thiophenes naphtho-furans and quinolines, L-ascorbic acid derivatives, phenanthridinium-bis-nucleobase conjugates, nucleoside analogues, hydantoin derivatives, crown ethers as well as diclofenac and fenoprofen thiolated and nonthiolated polyaspartamide-drug conjugates, were screened *in vitro* for potential antitumor activity and the possible mechanisms of action were ascertained for the most effective ones.

### Patents

P20050806A: Karminski-Zamola G; Hranjec M; Kralj M; Pavelić, K. Synthesis, photochemical synthesis and antiproliferative activity of cyano- and amidino-substituted 2-styryl benzimidazoles and benzimido[1,2-a]quinolines.

US patent: 7, 074, 437. Bašić R, Hadžija M, Subotić B. Mineral-protein preparations (MPP) and neuropathies in diabetes.

### Novel COST Project

Within the Domain of Biomedicine & Molecular Biosciences of the European Cooperation in the field of Scientific and Technical Research (COST) the new project proposed by Neven Žarković was launched in Brussels on June 2<sup>nd</sup>. This is the only COST project chaired by Croatian researchers.

The COST B35 Action denoted Lipid Peroxidation Associated Disorders: LPO tends to improve the understanding, monitoring

and control of LPO in medicine and biomedical research. To achieve these goals more than 160 researchers from 23 countries are developing the interdisciplinary network involving so far 35 research teams. The project will last for four years and is focused on four major research topics carried by the COST B35 work groups: 1) Improvement of methods for the determination of LPO products; 2) Studies of the fundamental aspects of LPO; 3) Pathological aspects of LPO and 4) Development and validation of antioxidants. For further information please visit the B35 web-site <http://www.irb.hr/costb35/>.

### International recognition

Kresimir Pavelic was re-elected as the vice-president of the European Molecular Biology Conference (for the 3<sup>rd</sup> time). Kresimir Pavelic is also a member of the Standing Committee of the European Medical Research Council, the European Science Foundation, the Council of the European Molecular Biology Laboratory and the Strategic Working Party of the European Molecular Biology Organization.



Figure 4. European Molecular Biology Laboratory countries



## Modern facilities, methods and equipment

The unit for Neurodegenerative Disease Research was established, led by Silva Hećimović. The main research interests are the molecular and cellular mechanisms of dementias, in particular Alzheimer's disease, and the role of cholesterol in Alzheimer's disease. This research is supported by the NIH-Fogarty International Research Collaboration Award, and a collaborative research grant supported by DAAD.

## Education

The Division provides over 50 undergraduate and 5 graduate courses at Universities in Zagreb, Rijeka, Dubrovnik and Osijek annually. 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>).

In 2006 joint PhD studies of Ruđer Bošković Institute, University of Osijek and University of Dubrovnik began in the field of Molecular Biosciences ([www.unidu.hr/molekularna/index.html](http://www.unidu.hr/molekularna/index.html)). More than thirty students from all regions of the Croatia signed for studies in 2006, while the first workshop denoted "Mentorship Fair" organised to provide mentors for all students was held at the Institute in September 2006.

In parallel the agreement on joint PhD studies was also signed with Universities of Split, Zadar and Dubrovnik. The PhD study on "Biology of Neoplasm" began to sign students in autumn 2006 expecting to start in 2007.

## AWARDS

Award to Sanja Kapitanović: The Croatian State Reward, the most prestigious scientific

recognition available in Croatia, was given to Sanja Kapitanović, senior scientist at the Division of Molecular Medicine. Sanja Kapitanović was awarded for the research in field of biomedicine.

## PROJECTS

### Projects supported by the Ministry of Science, Education and Sports

1. Molecular mechanisms in the pathogenesis of neuroendocrine tumours, Koraljka Gall-Trošelj
2. Molecular genetics of gastrointestinal tumours, Sanja Kapitanović
3. The SHH/PTCH/SMO signalling pathway in cancer and development, Sonja Levanat
4. Role of FHIT in neuroendocrine tumours, 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. Cxcl12/Cxcr4: new target for chemoprevention and treatment of colon tumours, Radan Spaventi
11. Molecular mechanisms of immunosuppression, Renata Novak
12. Modulation of immunological response by bioactive peptides, Biserka Pokrić
13. Tumour gene therapy – correction of oncosuppressor genes, Jasminka Pavelić
14. Virus antitumorous action and oncolytic virus vaccine, Mislav Jurin
15. Embryonic cell production of pancreatic-like islets, Mirko Hadžija
16. DNA chip technology in global profiling of tumours, Šime Spaventi
17. Nonlinear modulation of the chronic lymphatic leukaemia, Branko Vitale
18. Regulation of ectopeptidases and opioid receptors expression, Jelka Gabrilovac

19. Oxidative/antioxidative status after treatment with opioids/opiates, Tatjana Marotti
20. Neuropharmacology of serotonergic system, Dorotea Mueck-Šeler
21. Neurotransmitters in stress and regulation of GABA-A receptors in vitro, Danka Peričić
22. Assessing functions of the heat repeat in Huntington protein, Oliver Vugrek
23. The effects of new drugs and hyperthermia on the growth of mouse tumours and human xenografts, Marko Radačić
24. Immune interactions and immunomodulation in genital herpes infection, Zorka Mikloška

### **Research, developmental and international projects**

1. Centre for integrative genomics, molecular diagnostics, cellular and gene therapy, Krešimir Pavelić (MZOŠ, JEZGRA, J-1-2004)
2. Development a new and improved vaccine against genital herpes, Zorka Mikloška (MZOŠ, HITRA, TP-03/0098-39)
3. Molecular genetic background of Gorlin syndrome, Sonja Levanat (Bilateral Cooperation "Cogito", Bordeaux, France)
4. Developing method for detection of inherited predisposition to breast cancer in Croatia, Sonja Levanat (MZOŠ, HITRA, TP-07/009840)
5. Application of macromolecular derivate (G-90) from *Eisenia foetida* in biomedicine, Mira Grdiša (MZOŠ, HITRA, TP-03/009841)
6. Involvement of the ESCRT machinery in TfR sorting towards HD3 exosomes. Mira Grdiša (Cogito)
7. Bioactive properties of domestic pollen from *Salix alba* and *Cistus* sp. Tanja Marotti (HITRA, TP-05/0098-49).
8. Therapeutical effects of medicinal mushrooms. Mislav Jurin (HITRA, E60/2006)
9. The role of cholesterol in Alzheimer's disease, Silva Hećimović (Fogarty International Research Collaboration Award- NIH, USA, 1R03TW007335-01)
10. COST (European Cooperation in the field of Scientific and Technical Research) Action B35 "Lipid Peroxidation Associated Disorders" in the Domain Biomedicine and Molecular Biosciences, Action Chair Neven Žarković
11. Effects of the Lipid Peroxidation Product 4-Hydroxynonenal on Primary Hepatocytes,

Croatian-Austrian Science Technology Co-operation Program, Neven Žarković

### **SELECTED INVITED LECTURES**

1. Pivac N, Kozarić-Kovačić D, Muck-Šeler D, Mustapić M, Deželjin M: Neurobiology of PTSD in International NATO workshop u Centre of Excellence defence against terrorism. Integration of people experience trauma after terrorist attacks into modern society. Ankara, Turkey, April 27-28, 2006.
2. Pivac N: Neurobiological basis and treatment of PTSD. NATO Workshop "Human and Societal Dynamics: Activities of NATO SCOM in Pfp Countries of W. Balkan" organized by Ministry of Higher Education, Science and Technology of Slovenia and NATO SCOM. In: Ljubljana, Slovenija, May 29, 2006.
3. Žarković N: Role of COST in the European Research Area- Insight on projects in the field. The United Kingdom Royal Society's & Ministry of the European Parliament Scientist Pairing Scheme Meeting, Brussels, June 1, 2006.
4. Borović S: Enzyme-linked immunosorbent assay for 4-hydroxynonenal-histidine conjugates. 3rd International Meeting of the HNE-Club Genoa, Italy, June 16-18, 2006.
5. Čipak A: Possible involvement of 4-hydroxynonenal in splenocyte regulated liver regeneration. International conference of international medical association for experimental and clinical research, Progress in Liver Diseases, Lendava, Slovenia, September 21-23. 2006
6. Pavelić K: Integrative genomics in research and treatment of breast cancer. 14<sup>th</sup> World congress on breast cancer. Zagreb, Croatia, May 18-21, 2006.
7. Pavelić J: Bioethical aspects of gene therapy. In 2<sup>nd</sup> Sudeuropeisches Bioethik Forum, Mali Lošinj, Croatia, June 15-17, 2006.
8. Pavelić J: Molecular medicine: basic knowledge. In: 1<sup>st</sup> International Summer School "Integrative Bioethics" Mali Lošinj, Croatia, September 4-16. 2006.
9. Levanat S: Signal transductions in tumors: Hh-Gli interactions and therapeutic potential. In: 11<sup>th</sup> World Congress on Advances in Oncology and 9<sup>th</sup> International Symposium on



Molecular Medicine, Crete, Greece, October 12-14, 2006.

10. Čretnik M: Methylation status of PTCH promoter in tumours with alterations in Hh-Gli signalling pathway. In 11<sup>th</sup> World Congress on Advances in Oncology and 9<sup>th</sup> International Symposium on Molecular Medicine, Crete, Greece. October 12-14, 2006.
11. Musani V: Physiological significance of polymorphisms in BRCA 1 and 2. Difference in melting profile reflecting polymorphic or mutational variability. In: 11<sup>th</sup> World Congress on Advances in Oncology and 9<sup>th</sup> International Symposium on Molecular Medicine, Crete, Greece, October 12-14, 2006.
12. Levanat S: Molecular signalling in Breast Cancer. In: 14<sup>th</sup> World Congress on Breast Diseases, Zagreb, Croatia, 18-21, May, 2006.

## SELECTED PUBLICATIONS

1. Majhen D, Gabrilovac J, Eloit M, Richardson J, Ambriović-Ristov A: Disulfide bond formation in NGR fibre-modified adenovirus is essential for retargeting to aminopeptidase. *Biochem Biophys Res Com* 2006: 348: 278.
2. Čipak A, Hasslacher M, Tehlivets O, Collinson E J, Živković M, Matijević T, Wonisch W, Waeg G, Dawes I W, Žarković N, and Kohlwein S.D: *Saccharomyces cerevisiae* strain expressing a plant fatty acid desaturase produces polyunsaturated fatty acids and is susceptible to oxidative stress induced by lipid peroxidation. *Free Radical Biol Med* 2006: 40: 897.
3. Prutki M, Poljak-Blaži M, Jakopović M, Tomas T, Stipančić I, Žarković N: Altered iron metabolism, transferrin receptor 1 and ferritin in patients with colon cancer. *Cancer Lett* 2006: 238: 188.
4. Biasi F, Vizio B, Mascia C, Gaia E, Žarković N, Chiarpotto E, Leonarduzzi G, Poli G: JNK up-regulation as a key event in the pro-apoptotic interaction between TGF- $\beta$ 1 and 4-hydroxynonenal in colon mucosa. *Free Radical Biol Med* 2006: 40: 443.
5. Belužić R, Ćuk M, Pavkov T, Fumić K, Barić I, Mudd SH, Jurak I, Vugrek O: A single mutation at tyrosine 143 of human S-adenosylhomocysteine hydrolase renders the enzyme thermosensitive and effects the oxidation

state of bound co-factor NAD. *Biochemical J* 2006: 400: 245.

6. Pavelić K, Dedivitis RA, Kapitanović S, Čačev T, Guirado CR, Danić D, Radošević S, Brkić K, Pegan B, Križanac S, Kusić Z, Spaventi S, Bura M: Molecular genetic alterations of FHIT and p53 genes in benign and malignant thyroid gland lesions. *Mutation Res* 2006: 599: 45.
7. Pivac N, Kozarić-Kovačić D, Mustapić M, Deželjin D, Borovečki A, Grubišić-Ilić M, Muck-Šeler D: Platelet serotonin in combat related posttraumatic stress disorder with psychotic symptoms. *J Affect Disord* 2006: 93: 223.
8. Šagud M, Mihaljević-Peleš A, Muck-Šeler D, Jakovljević M, Pivac N: Quetiapine augmentation in treatment-resistant depression: a naturalistic study. *Psychopharmacology* 2006: 187: 511.
9. Grbeša I, Ivkić M, Pegan B, Gall-Trošelj K: Loss of imprinting and promoter usage of the IGF2 in laryngeal squamous cell carcinoma. *Cancer Lett* 2006:238: 224.

## Review articles

1. Kraljević S, Sedić M, Scott M, Gehring P, Schlapbach R, Pavelić K: Casting light on molecular events underlying anti-cancer drug treatment: What can be seen from the proteomic point of view? *Cancer Treat Rev* 2006: 32: 619.
2. Fontana S, DeLeo G, Sedec M, Kraljević Pavelić S, Alessandro R: Proteomics in anti-tumor research. *Drug Discovery Today* 2006: 3: 441.
3. Pavelić J, Matijević T, Knežević J: Fetal gene therapy: current prospects. *Curr Stud Biotechnology* 2006: 4: 77.
4. Kralj M: Molecular-targeted approach to cancer therapy – the roles of p53 and p21 WAF1/CIP1 genes. *Curr Stud Biotechnology* 2006: 4: 27.
5. Pavelić K, Primorac D, Vuk-Pavlović S: Integrating new countries into the European Research Area. *EMBO Rep* 2006: 7 : 458.
6. Levanat S, Musani V, Levačić-Cvok M, Čretnik M: Molecular signalling in Breast cancer. *Medimond International Proceedings*, Medimond S.r.l., Moduzzi Editore, 2006: ISBN 88-7587-292-9, 7-12.

## Chapters in books

1. Kozarić-Kovačić D, Pivac N. Psychotic features of combat related chronic posttraumatic stress disorder and antipsychotic treatment. In: Novel approaches to the diagnosis and treatment of posttraumatic stress disorder. NATO Security through Science series E: Human and Societal Dynamics – Vol 6. IOS Press Amsterdam Berlin Oxford Tokyo Washington DC. , Section 1: Epidemiology and pathophysiology of PTSD, 2006: 42-55.
2. Pivac N, Kozarić-Kovačić D, Mück-Šeler D. Biological markers in Croatian war veterans with combat related posttraumatic stress disorder. In: Novel approaches to the diagnosis and treatment of posttraumatic stress disorder. NATO Security through Science series E: Human and Societal Dynamics – Vol 6. IOS Press Amsterdam Berlin Oxford Tokyo Washington DC., Section 1: Epidemiology and pathophysiology of PTSD, 2006 3 - 12.



# Division of Marine and Environmental Research

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

## DIVISIONAL ORGANIZATION

Head: Tarzan Legović

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

- ⇒ Group for satellite oceanography, Milivoj Kuzmić
- ⇒ Group for modelling and information systems, Ivica Ružić
- ⇒ Laboratory for physico-chemical separations, Zlatica Kozarac
- ⇒ 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, Tarzan Legović



## OVERVIEW OF THE ACTIVITY DURING 2006

During 2006, scientists of the division worked on 61 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 interplanetary ecology and satellite oceanography down to nanotechnology. Each project contributed to the overall mission of the division: 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 optimum management of the environment and hence the benefit of our country and, indeed, the whole world.

The research results were published in 44 scientific papers in journals indexed by Current Contents. In addition, one patent was filed, 12 invited lectures were held and 3 conferences were organized under the auspices of the Division. Also, 5 study programs were coordinated, 5 M.Sc. and 5 Ph.D theses were

defended, one book was published, 22 CDs of teaching materials were completed. Finally, 10 undergraduate and 38 post-graduate courses were given at universities in Croatia and abroad.

## TOP ACHIEVEMENTS

### **New methods for determination xenobiotic chemicals and effect-directed analyses of municipal wastewaters**

Highly specific methods based on high-performance liquid chromatography coupled to tandem mass spectrometry (LC/MS/MS) and gas chromatography-mass spectrometry (GC/MS) were developed for the determination of several groups of environmental contaminants, including 3 major classes of antimicrobials, alkylphenolic endocrine-disrupting compounds and polycyclic aromatic hydrocarbons and their hydroxylated metabolites. For the first time, the organic toxicants present in the effluent of the main sewer of the city of Zagreb, were isolated and identified through the use of effect-directed characterisation techniques.

### **Determination of new mixed ligand complex iron(III)-glycin-NTA**

Dissolved iron has a crucial role in the primary production processes of the aquatic environment. Hence, numerous complexes of ionic iron were investigated. New mixed ligand complex iron(III)-glycin-NTA was determined, stable in the solution over 24 hours at seawater pH (~8), with concentration of iron several orders of magnitude higher than in natural waters that secures enhanced iron bioavailability (Cuculić V. and Pižeta I, Croat Chem Acta 2006:79: 41).

### **Electrochemical impedance spectroscopy for characterization of sea surface microlayer**

Boundary areas between different environmental compartments represent critical interfaces of special biological, chemical and physical properties. The exchange of matter and energy between water and atmosphere has a decisive role in global changes and in environmental protection. The sea surface microlayer (SSM) represents the boundary layer between the sea and the atmosphere and is derived from multiple sources and



Figures 1, 2: Sampling for the Projects "Determination of ecotoxic trace metals in water, sediment and biota of NP Mljet" and "Geochemistry of ecotoxic metals in the region of NP Krka".



composed of different natural and anthropogenic organic substances. For the first time electrochemical impedance spectroscopy (EIS) was used for physico-chemical characterization of SSM. The results give information on the polarity and structural homogeneity of the microlayer and provide a method of distinguishing different microlayer samples (Frka S et al., Int J Environ Anal Chem 2006: 86: 325).

### **Melanoidins as a key link in the transformation of polysaccharides to humic material in the marine environment**

Melanoidins, which are condensation products of sugars and amino acids, represent a key link in the transformation of polysaccharides to humic material in the marine environment. The copper complexing properties of prepared melanoidins and humic material isolated from marine lagoon sediments were measured. The presence of other micro- and macroconstituents in seawater influences their complexing properties towards metal ions (Plavšić M et al., Sci. Total Environ, 2006: 366: 310).

### **Dissolved copper and cadmium partitioning in coastal areas of the Aegean Sea**

Dissolved copper and cadmium partitioning and their complexation with organic matter were investigated in shallow coastal areas of the Aegean Sea (Eastern Mediterranean). The percentage of DGT-labile copper as for total dissolved copper ranged from 13 to 34% during summer and from 23 to 36% during winter, whereas the corresponding percentage for DGT-labile cadmium was higher in summer (38 to 68%), in comparison to winter (29 to 44%). The mean value of transparent exopolymeric particles in summer was high (208 µg/L xanthan equiv.), while in winter it reached 441 µg/L xanthan equiv., which indicates significant phytoplankton activity

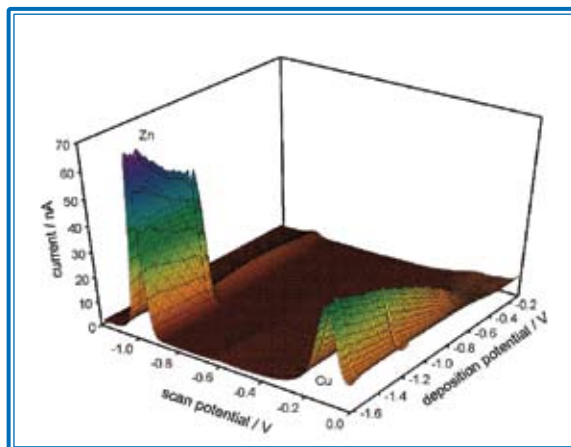


Figure 3: Pseudopolarograms as voltammetric "fingerprints" of a water sample to determine dissolved trace metal speciation

in winter. A significant fraction of dissolved organic carbon (DOC) is surface active and was determined. Carbohydrates were also determined and they represented up to 33% of the DOC (Scoullou M et al., Estuar Coast Shelf Sci 2006: 67: 484).

### **Quality of peloid in Morinje termed exceptional**

Research on the geochemical features and medicinal properties of peloid muds from the Morinje bay, near Šibenik, on the Croatian Adriatic coast showed that the quality of the material is exceptional. The report will be used as a feasibility study for the establishment of health tourism in the area, and for environmental protection measures at the site. (Mihelčić G et al., Croat Chem Acta 2006: 79: 161).

### **Microflora of bluefin tuna**

Gram-negative bacteria from genera *Moraxella*, *Pasteurella*, *Brevundimonas*, *Weeksella*, *Klebsiella* and *Pseudomonas* dominated the microflora on examined tuna, whereas *Staphylococcus* was the only Gram-positive isolated genus (Kapetanović et al., Aquaculture Res 2006: 37: 1265).

## Patent

Svetličić V, Žutić V, Hozić Zimmermann A. Amperometric method and apparatus for measurement of soft particles in liquids by analysing the adhesion of these particles to an electrode. International application No. PCT/HR2006/000008.

## EDUCATIONAL ACTIVITIES

### Oceanography

Since 1971, an interdisciplinary M.Sc. course in cooperation with the University of Zagreb. During 2005 the course was upgraded to the Ph.D. level. Čosović B.

### Environmental protection and nature conservation

Since 2001 an interdisciplinary M.Sc. course in cooperation with the University J.J. Strossmayer, Osijek. During 2006 the course was upgraded to the Ph.D. level. Čosović B.

### Environmental management (an international course)

Since 2003 a Ph.D. granting course in cooperation with the University of Zagreb. Legović T.

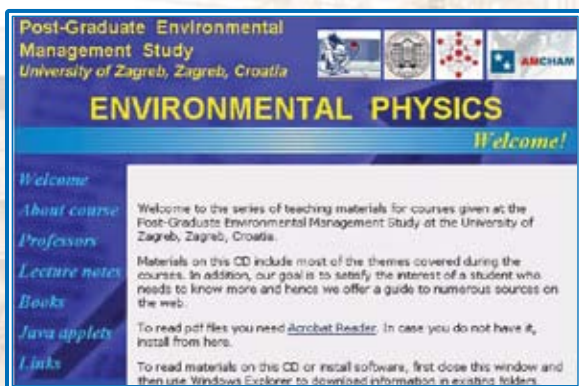


Figure 4: Environmental Physics. One of 22 CDs developed for the Post Graduate Environmental Management Study.

## Biophysics

University of Split, Svetličić V.

### Regional Advanced Training Course, IAEA

Sampling, sample preparation and analysis for the measurement of radionuclides in the marine environment was performed in Rovinj, 02 - 12 May 2006. (Scientific director Lulić S.)

## NOMINATIONS AND AWARDS

1. Legović T. Secretary General, International Society for Ecological Modelling.
2. Filipović Marijić V. Metal exposure assessment in native fish, *Mullus barbatus L.*, from the Eastern Adriatic sea, Highly Commended Poster. European Societies of Toxicology Annual Congress, 20-24 September 2006 Croatia.

## PROJECTS

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

1. Tidal and longer-period dynamics of the northern Adriatic, Milivoj Kuzmić
2. Models and info. systems for environmental protection and navigation management, Ivica Ružić
3. Electroanalytical research in liquid and solid electrolytes, Milivoj Lovrić.
4. Preparation and properties of metal surfaces in the environmental protection, Dunja Čukman
5. Radionuclides in environmental systems, Delko Barišić
6. Interfacial processes and eutrophication, Vera Žutić
7. Physical chemistry and biogeochemistry of trace metals in aquatic systems, Ivanka Pižeta.



8. Geochemistry of recent and ancient sedimentary systems of the Adriatic platform, Goran Kniewald
9. Nature and reactivity of organic substances in seawater and environment, Božena Čosović
10. Analysis and biogeochemistry of organic compounds in the aquatic environment, Marijan Ahel
11. Persistent organohalogen pollutants in some coastal area of Dalmatia, Mladen Picer
12. Metals and cellular biomarkers, Biserka Raspor
13. Microbial communities as catalysts in biotransformation processes, Dubravka Hršak
14. Multixenobiotic resistance mechanism as a biomarker of environmental quality, Tvrtko Smital
15. Protection of biocoenotic balance in aquaculture receiving waters, Emin Teskeredžić
16. Modelling aquatic ecosystems, Tarzan Legović

### **Selected projects for outside clients**

1. Reduction of environmental risks, posed by emerging contaminants, through advanced treatment of municipal and industrial wastes (EMCO) EU-FP6 Project, 2004-07, Marijan Ahel
  2. Sava River Basin: Sustainable use, management and protection of resources (SARIB). EU FP6, 2004-06, Biserka Raspor
  3. Ecosystem Approach for Sustainable Aquaculture (ECASA). EU-FP6, 2005-07, Tarzan Legović
  4. Electrochemical characterization of marine polysaccharides, Deutsche Forschungsgemeinschaft, Marta Plavšić and U Passow.
  5. Marine science and coastal management in the Adriatic Western Balkan, An education and research network, Norwegian cooperation Programme on Research and Higher Education. Božena Čosović and P Wasman.
  6. Novel physical chemical techniques to characterize the sea surface microlayer, The Royal Society UK, Zlatica Kozarac and A Nelson.
7. Reference Laboratory, Ministry of Agriculture, Forestry and Water Management, Water Management Directorate. Božena Čosović, Dubravka Hršak, Zlatica Kozarac and Biserka Raspor.
  8. Taxonomic, genetic and physiological characterization of bacteria for atrazine degradation, French-Croatian bilateral COGITO project, 2005-2006, Dubravka Hršak.
  9. Formation of recent carbonates in karstic environments. Croatian-Slovenian Collaboration Project. Ivica Sondi.
  10. Monitoring of Danube water quality, Croatian Waters, Stipe Lulić.
  11. Development of field method for gross alpha activity of radon and thoron in soil gas. Croatian-Slovenian bilateral cooperation, Delko Barišić.
  12. Determination of trace metals in fresh, brackish and sea waters of Republic Croatia, Croatian Water Agency, 2006-10, Marina Mlakar.
  13. Ecotoxic metals in aquatic organisms of national park «Plitvice lakes», NP Plitvice lakes, 2005-07, Dario Omanović.
  14. Determination of ecotoxic trace metals in water, sediment and biota of National Park Mljet, NP Mljet, 2006-07, Vlado Cuculić.
  15. Geochemistry of ecotoxic metals in the region of NP Krka, NP Krka, 2005-8, Neven Cukrov.
  16. Economical bases of Korana, Dobra, Mrežnica, Kupa and Una Rivers, streams Dabar, Jaruga, Matica and Krbavica. Emin Teskeredžić.
  17. The Electronic Information Panels at two Bridges near Ilok and Batina, Putting in Operation, Croatian Agency of inland fairways with CRUP d.o.o, 2006, Zagreb. Ivica Ružić



Figure 5: Panel at the bridge across the Danube River near Ilok showing water depth in cm.

## SELECTED INVITED LECTURES

1. Ahel M. Sampling strategies to study organic contaminants in municipal wastewaters, COST 636 "Xenobiotics in the Urban Water Cycle", Annual meeting, Vienna, Austria, September 25-27, 2006.
2. Kozarac Z. Electrochemical and monolayer studies of lipid interaction with heavy metals and organic pollutants, Meeting of Consortium BBMO (Biosensors based on molecular organization), Strömbäck, Sweden, June 8, 2006.
3. Legović T. Environmental carrying capacity for aquacultures, Institute for Marine Science, University of the Philippines, Manila, Philippines, November 27, 2006.
4. Pižeta I. Working electrodes in voltammetry: from mercury macroelectrodes to solid microelectrodes, 4th Croatian Symposium on Electrochemistry, Primošten, Croatia, 28 May – 1 June 2006.
5. Svetličić V, Žutić V. Strings and Beads Produced by Marine Diatom *Cylindrotheca fusiformis*. Seeing at the Nanoscale IV, An International Conference. Philadelphia, Pennsylvania, USA. July 17 – 20, 2006.
6. Smital T. Inhibitors of the ABC Transport Proteins as Emerging Pollutants - Determination and Ecotoxicological Relevance. EUROTOX 2006/6CTDC Congress (43rd Congress of the European Societies of Toxicology and 6th Congress of Toxicology in Developing Countries), Cavtat/Dubrovnik, Croatia, September 20-24, 2006.

## ORGANIZED CONFERENCES

1. 4<sup>th</sup> Croatian Symposium on Electrochemistry, Primošten, 28 May – 1 June 2006 (Kozarac Z and Gašparović B.).
2. First Annual Meeting "Marine science and coastal management in the Adriatic Western Balkan, An education and research network", Kotor September 20-24, 2006 (Čosović B, Wassmann P and Krivokapić S).
3. Christmas Biophysics Workshop, Zagreb, Croatia, December 18, 2006. (Svetličić V, president, Croatian Biophysical Society).

## VISITS

1. Prof. G.R. Helz, Department of Chemistry and Biochemistry, University of Maryland, USA through Fulbright Foundation, 01. February until 01. July 2006.
2. Prof. Ewen McLean, Ph.D., VTAC Department of Fisheries and Wildlife Sciences, Blacksburg, VA, USA 5-9 June 2006.
3. Dr. Tin Klanjšček, Post doctoral fellow, Massachusetts Institute of Technology, Cambridge and Woods Hole Oceanographic Institution, Woods Hole, MA, USA, July 2006 -July 2007.

## SELECTED PUBLICATIONS

1. Cuculić V, Pižeta I: Electrochemical characterisation of Iron(III)-Glycine-Nitrilotriacetate mixed ligand complexes and their stability in aqueous solution. Croat Chem Acta 2006: 79: 41.
2. Garnier C, Lesven L, Billon G, Magnier A, Mikkelsen O, Pižeta I: Voltammetric procedure for trace metal analysis in polluted natural waters using homemade bare gold-disk microelectrodes. Anal Bioanal Chem 2006: 386: 313.
3. Grahek Ž, Rožmarić Mačefat M, Lulić S: Isolation of lead from water samples and determination of 210-Pb. Anal Chim Acta 2006: 560: 84.
4. Horvat-Radošević V, Kvastek K: Role of Pt-probe pseudo-reference electrode in impedance measurements of Pt and polyaniline (PANI) modified Pt electrodes. J Electroanal Chem 2006: 591: 217.
5. Janeković I, Antonić O, Križan J, Bukovec D, Bakran-Petricoli T: Modelling basic physical parameters in the Adriatic Sea as the basis for marine habitats mapping. Ecol Modelling 2006: 194: 62.
6. Krznarić D, Helz GR, Ciglencečki I: Prospect of determining copper sulfide nanoparticles by voltammetry: A potential artifact in supersaturated solutions. J Electroanal Chem 2006: 590: 207.
7. Mandić Z, Gašparović B, Weitner Z: Electrochemical Reduction of Rh(bpy)(3+)(3) at



- Hg/Phosphate Electrolyte Interface. *J Electroanal Chem* 2006: 587: 314.
8. Mihelčić G, Lojen S, Dolenec T, Kniewald G: Trace Metals Conservation in Morinje Bay Sediment: Historical Record of Anthropogenic Immissions into a Shallow Adriatic Bay. *Croat Chem Acta* 2006: 79: 161.
  9. Oreščanin V, Mikelić L, Roje V, Lulić S: Determination of lantanides by source excited EDXRF method after preconcentration with APDC. *Anal Chim Acta* 2006: 570: 277.
  10. Pivčević B, Žaja R: Pesticides and their binary combinations as p-glycoprotein inhibitors in NIH 3T3/mdr1 cells. *Environ Toxicol Pharm* 2006: 3: 268.
  11. Scoullou M, Plavšić M, Karavoltzos S, Sakellari A: Partitioning and distribution of dissolved copper, cadmium and organic matter in Mediterranean marine coastal areas: The case of mucilage event. *Estuarine Coastal Shelf Sci* 2006: 67: 484.
  12. Plavšić M, Čosović B, Cindy L: Copper complexing properties of melanoidins and marine humic material. *Sci Total Environ* 2006: 366: 310.





# Centre for Marine Research

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

## DIVISIONAL ORGANISATION

Head: Nenad Smodlaka

The Centre for Marine Research consists of the following laboratories:

- ⇒ Laboratory for ecology and systematics, Ana Travizi
- ⇒ Laboratory for processes in the marine ecosystem, Danilo Degobbi
- ⇒ Laboratory for ecophysiology and toxicology, Čedomil Lucu
- ⇒ Laboratory for marine molecular toxicology, Renato Batel
- ⇒ Laboratory for ecotoxicology, Bartolo Ozretić



atic Sea. The mechanisms of eutrophication, hypoxia and anoxia, as well as the recently very frequent mucilage events in the region, are also under investigation. Regarding applied research, efforts are being focused towards implementing the widely accepted concept of the Coordinated Adriatic Observing System (CAOS), in collaboration with all the relevant research institutions and authorities from the Adriatic-bordering states. The Croatian input to CAOS is the National Monitoring Program (Project "Jadran") which has been coordinated by the Centre since 1998. The Centre is also engaged in the education of young scientists at the postgraduate level in oceanology and geophysics at the University of Zagreb.

## OVERVIEW OF THE CENTRE

The Centre for Marine Research in Rovinj is the only department of the Ruđer Bošković Institute located outside of the main campus in Zagreb. The mission of the Centre includes both basic research of processes in the marine environment and applied studies, related to the main environmental problems in the Adriatic Sea, for the Croatian Government, local authorities, various companies and other institutions. Processes are studied from the cellular level, mainly focused on sub-lethal effects of pollutants and other environmental factors on marine organisms, to the regional scale, principally seasonal and long-term changes in the plankton communities and benthos of the northern Adri-

## TOP ACHIEVEMENTS

### Preconditioning processes of winter thermohaline conditions in the northern Adriatic

An analysis of the 1966-2000 data showed that February thermohaline characteristics depend on meteorological and hydrological processes which occur during the autumn, spring and even winter of the preceding year (Supić N et al., *Estuar Coast Shelf Sci* 2006: 66: 580).

## Mechanism of autumnal Po waters spreading over the northern Adriatic

In autumnal situations of increased fresh-water input, Po River waters were likely to reach the Istrian coast in conditions of prolonged SE or SW winds. They remained confined to the western part of the basin in conditions of prevailing E or NE winds (Supić N et al., Fresen Environ Bull 2006: 15: 193).

## Warming trend in the northern Adriatic

Studies of long-term oceanographic data by new statistical methods indicated a warming trend of about 1 °C at the surface and of about 0.6 °C at the bottom over the past 38 years, and may be consistent with global warming estimates (Figure 1; Lyons et al., Acta Adriat 2006: 47: 81).

## Microbial heterotrophic activity along the gradients

The importance of the “top-down” control

of heterotrophic bacteria by heterotrophic predation of nanoflagellates declines spatially from the eastern to the western part of the Rovinj – Po Delta profile, and temporally from 1990 onwards, indicating an increase of eutrophication. The availability of Inorganic nutrients for bacterioplankton production and degradation of TEP and CSP is an important issue in organic matter accumulation in the northern Adriatic, predominantly phosphorus limited (Radić T et al., FEMS Microbiol Ecol 2006: 58: 333).

## Spontaneous regression of *Caulerpa taxifolia* (Vahl) C. Agardh from the northern Adriatic Sea

Apparently a spontaneous regression of the *C. taxifolia* settlement in the coastal area of Malinska was recorded in the 2000-2005 period (Figure 2) and recently has resulted in the extinction of the species in the northern Adriatic Sea (Iveša Lj et al., Aquatic botany 2006: 85: 324).

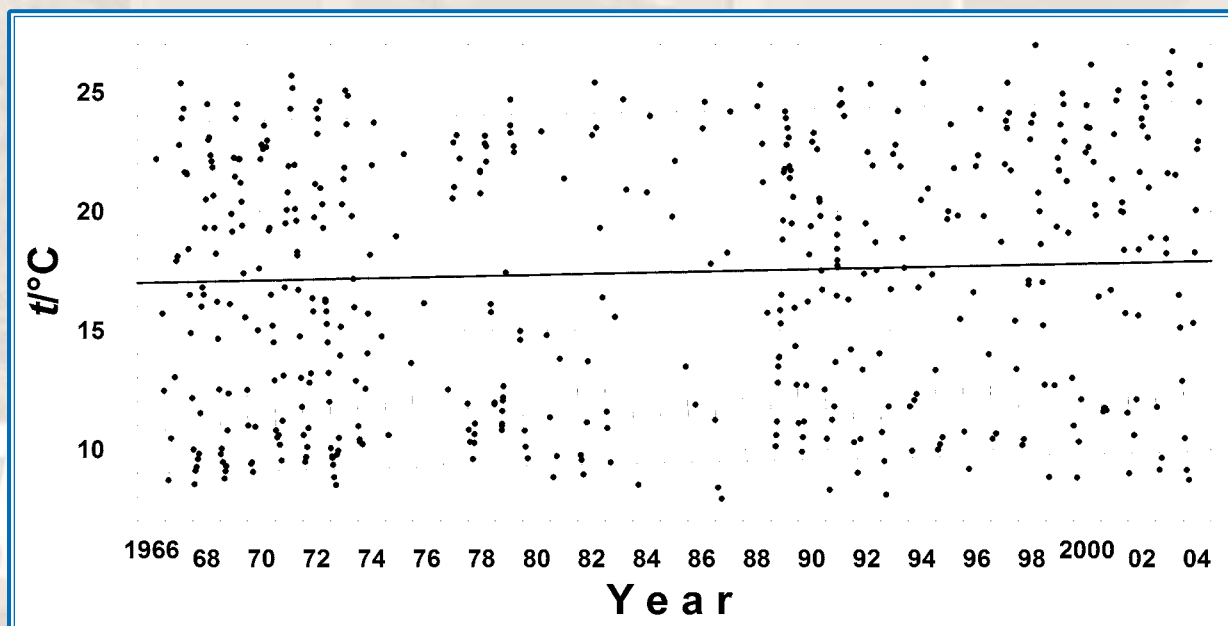


Figure 1. Surface temperature data, model fit, and linear trend for waters off Rovinj.



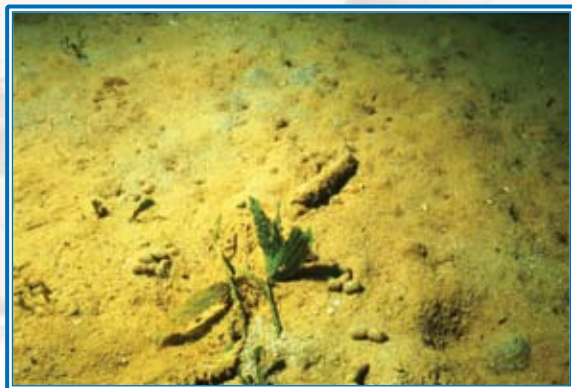


Figure 2. *C. taxifolia* settlement at Malinska – terminal phase of regression.

### Imposex in *Hexaplex trunculus* snails

High tributyltin (TBT) contamination in the northern Adriatic from antifouling paints were registered in the soft tissue of marine invertebrates ( $238.61 \pm 32.04 \text{ ng Sn g}^{-1}$  up to  $3223 \pm 333 \text{ ng Sn g}^{-1}$ ) (Garaventa et al., Develop Hydrobiol: 2006: 183: 281). TBT causes genetic disorder called “imposex”, a serious deformation of the endocrine system leading to the development of male sex characteristics in female *H. trunculus* snails (Garaventa et al., Hydrobiologia: 2006: 555: 281).

### Morphological changes in the oyster *Ostrea edulis* shells

An extremely low level of TBT in the seawater significantly affects shellfish larval growth, impairs the immune system of organisms, and cause malformations and mineralogical changes in the inner nacreous layer of bivalve shells (Medaković et al., SIA: 2006: 38: 313).

### Ecology of the sponge *Suberites domuncula*

*Ex situ*, permanent contractions to approximately half their size can change the consistency of the sponge, form, canal

structure, water flow, including the disappearance of oscula (Figure 3). In the wild, *in situ* reversible contractions could have protective function by reducing water filtration, decreasing the input of harmful substances, and providing a mechanical strength shield against predators.

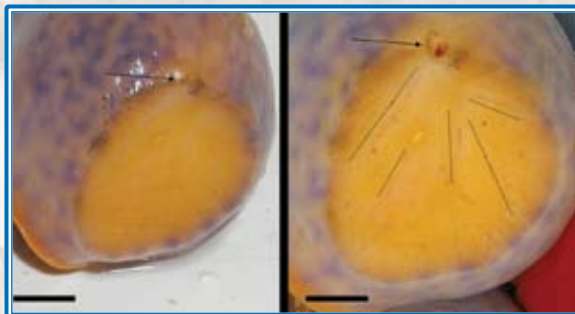


Figure 3. Cross sections of *S. domuncula* in proximity to the osculum: A) contracted and B) relaxed state. Bars represent 1 cm. Arrows reveal differences in osculum and dashed lines in channel contraction.

### Iroquois homeobox genes from *Suberites domuncula*

Three Iroquois homeobox genes from *S. domuncula* were identified and analysed (Figure 4). Two were shown to be active, the third one being a pseudogene. One of the active genes contains two homeodomains, the first time described among the Iroquois genes at all.

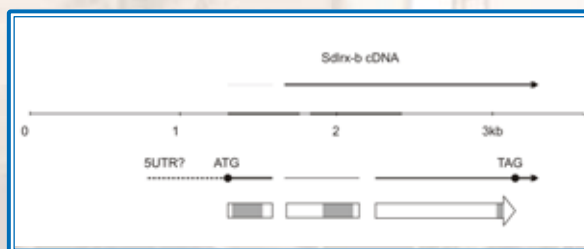


Figure 4. Schematic representation of the Iroquois gene locus coding for two homeodomains. The locus is 3.4 kb in length. Two duplicated regions containing the homeoboxes are bold. The deduced protein is shown at the bottom. Two homeodomains and the iro-box are shaded grey.

## Lobster excretory physiology

The role of the antennal gland in the urine ion-transport and osmoregulation in the commercially important Adriatic lobster *Homarus gammarus* was investigated. For the first time, in laboratory conditions, the enzyme  $\text{Na}^+, \text{K}^+$ -ATPase was found to be activated in the antennal lobster gland suggesting that it plays a role in hemolymph osmoregulation.

## PROJECTS

### Projects supported by the Ministry of Science, Education and Sports

1. Systematic research of the Adriatic Sea as a base for sustainable development of the Republic of Croatia, Project "Jadran", Croatian national monitoring programme, Nenad Smolaka
2. Mechanism of long-term changes in the Adriatic Sea ecosystem, Danilo Degobbis
3. Programmed biosynthesis and genotoxic risk assessments, Renato Batel
4. Physiological and biochemical indicators of toxicological stress in marine biota, Bartolo Ozretić
5. Ecophysiological studies and stress response in marine organisms, Čedomil Lucu

### Research, developmental and international projects

1. BiotecMarin, Molekulare Biotechnologie und Wirkstoffe Mariner Schwaemme sowie Schwamm-assoziiierter Mikroorganismen (Akronym: Kompetenz-zentrum «Biotec-Marin», Renato Batel, Werner. E.G. Müller (Croatian-German Cooperation in the Aquatic Field)

2. Biocapital (MCRTN), Cope with the challenges and opportunities of the 21<sup>th</sup> century: Integrated basic and applied training in a Success-oriented bioprospecting, Renato Batel, Werner E.G. Müller (EU-FP6)
3. Sponges, sustainable production, physiology, oceanography, natural products, genetics and economics of sponges, Renato Batel, Werner E.G. Müller (EU-FP6)
4. Realization of an integrated monitoring system of the quality of the Adriatic Sea, with particular regard to eutrophication and mucilage phenomena (REQUISITE), Danilo Degobbis (EU INTERREG IIIA, 2004-2006)
5. Integrated system for monitoring and forecasting of meteorological and water conditions parameters in the Adriatic Sea (ADRIAMET), Danilo Degobbis (EU INTERREG IIIA, 2004-2008)
6. Valutazione della sostenibilità di nuove strategie co-gestionali di pesca mediante un approccio ecosistemico (SosPEco), Danilo Degobbis (ICRAM, Rome, Italy, 2005-2006)
7. Molluscan biomineralization and embryonic development: molecular genetics of shell calcifying matrices, Davorin Medaković (Cogito Project 2005-2007)
8. Reproductive status and risk assessment of the European eel *Anquilla anquilla* from Balaton Lake (Hungary) and estuaries of the Adriatic Sea (Croatia) under different environmental conditions, Milena Mičić, Miklos Bercsenyi (Croatian-Hungarian scientific cooperation)
9. Anossie attuali nel Nord Adriatico, registrazione nei sedimenti in epoca storica, influenza sulle risorse di pesca e bentoniche. Modellizzazione e previsione (ANOCSSIA), Robert Precali (Ministero dell'Istruzione, dell'Università e della Ricerca della Repubblica Italiana, 2004-2007)
10. Adriatic Sea integrated coastal areas and river basin management system pilot project, ADRICOSM-EXT, Nenad Smolaka (UNESCO/IOC)



## SELECTED INVITED LECTURES

1. Degobbi D: Processes in the northern Adriatic water column. Regional Advanced Training Course on Sampling, Sample Preparation and Analysis for the Measurement of Radionuclides in the Marine Environment. International Atomic Energy Agency (IAEA), Rovinj, Croatia, May 2-12, 2006.
2. Medaković D: Pollution influence of the Adriatic ecosystem. Croatian Medical Council and Croatian Society for Healthy Ecology, Pula, Croatia, November 29, 2006.
3. Supić N: Physical oceanography of the Adriatic Sea. Regional Advanced Training Course on Sampling, Sample Preparation and Analysis for the Measurement of Radionuclides in the Marine Environment. International Atomic Energy Agency (IAEA), Rovinj, Croatia, May 2-12, 2006.
4. Travizi A: Sediments and Meiofauna of the Adriatic Sea. Regional Advanced Training Course on Sampling, Sample Preparation and Analysis for the Measurement of Radionuclides in the Marine Environment. International Atomic Energy Agency (IAEA), Rovinj, Croatia, 2-12 May 2006.
5. Travizi A: The 115<sup>th</sup> Anniversary of the Marine Research Station at Rovinj: Recent benthic research. 9<sup>th</sup> Croatian Biological Congress with International Participation. Croatian Biological Society. Rovinj, Croatia, September 23-29, 2006.

## SELECTED ORGANIZED CONFERENCES

IAEA (REF/7/003) Regional Advanced Training Course on Sampling, Sample Preparation and Analysis for the Measurement of Radionuclides in the Marine Environment. Rovinj, Croatia, May 2-12, 2006 (host institution Center for Marine Research in cooperation with the Laboratory for radioecology, RBI).

## SELECTED PUBLICATIONS

1. Garaventa F, Pellizzato F, Faimali M, Terlizzi A, Medakovic D, Geraci S, Pavoni B: ImPOSEX in *Hexaplex trunculus* at some sites on the North Mediterranean Coasts as a base-line for future evaluation of the effectiveness of the total ban on organotin based antifouling paints. *Hydrobiologia* 2006: 555: 281.
2. Garaventa F, Pellizzato F, Faimali M, Terlizzi A, Medakovic D, Geraci S, Pavoni, B: ImPOSEX in *Hexaplex trunculus* at some sites on the north Mediterranean coast as a base-line for future evaluation of the effectiveness of the total ban on organotin based antifouling paints. In: Queiroga, H. et al. (Ed.) *Marine biodiversity: patterns and processes, assessment, threats, management and conservation. Developments in Hydrobiology*, 2006: 281.
3. Iveša Lj, Jaklin A, Devescovi M: Vegetation patterns and spontaneous regression of *Caulerpa taxifolia* (Vahl) C. Agardh in Malinska (northern Adriatic, Croatia). *Aquatic Botany* 2006: 85: 324.
4. Medaković D, Traverso P, Bottino C, Popović S: Shell layers of *Ostrea edulis* as an environmental indicator of TBT pollution: the contribution of surface techniques. *Surface and Interface Analysis* 2006: 38: 313.
5. Radić T, Ivančić I, Fuks D, Radić J: Marine bacterioplankton production of polysaccharidic and proteinaceous particles under different nutrient regimes. *FEMS Microbiol Ecol* 2006: 58: 333.
6. Supić N, Vilibić I: Dense water characteristics in the northern Adriatic in the 1967-2000 interval with respect to surface fluxes and Po river discharge rates. *Estuar Coast Shelf Sci* 2006: 66: 580.
7. Supić N, Đakovac T, Krajcar V, Kuzmić M and Precali R : Effects of excessive Po River discharges in the northern Adriatic. *Fresen Environ Bull* 2006: 15: 193.
8. Lyons DM, Janeković I, Precali R, Supić N: Northern Adriatic Sea hydrographic conditions from October 2002 - September 2003, including the climatic heating anomaly of summer 2003. *Acta Adriat* 2006 Suppl: 47: 81.





## ORGANISATION OF THE CENTRE

Head: Karolj Skala

The Centre for Informatics and Computing (CIC) consists of the following departments:

- ⇒ Laboratory for Optoelectronics and Visualisation, Karolj Skala
- ⇒ ICST research and development, Zorislav Šojat
- ⇒ Information systems, Neven Kmetić
- ⇒ Service and maintenance, Ratko Mileta



project was the establishment of a national computing grid. CIR was the leader of the CRO-GRID Applications project and member of the CRO-GRID Infrastructure project. CIC continued further development of the Grid Portal, through which scientists are able to access the grid computing resources and submit complex compute-intensive jobs.

In the last year RBI, SRCE and Faculty of Electronics, Mechanical Engineering and Shipbuilding from Split jointly formed the CRO-GRID JRU (Joint Research Unit), and were accepted as a JRU partner into the EU FP6 EGEE-II project (presently the biggest computer oriented project in the world). Inside the CRO GRID JRU RBI/CIC is the JRU leader of NA2 (dissemination) and NA4 (Applications). Furthermore, CIR is actively collaborating in other work packages of the EGEE-II project. A lot of activities inside the two Networking Activities were very well accepted by the EGEE-II project consortium, e.g. the NA4 activity of "Grid Library Applications" development (i.e. PARF), the NA2 GridVision alternative scientific promotion initiative etc.

## OVERVIEW OF THE CENTRE

### Scientific Research and Development

During 2006, CIR continued the eScience programme based on ICST (Information Communication Science Technology) on Grid platforms. This programme is based on the National Grid Initiative poly-project CRO-GRID, which included 11 institutions and over 50 explorers. The goal of the poly-



Figure 1. CRO GRID Infrastructure

The successful reimplementation and parallelisation the random forests algorithm (PARF), was followed by the gridification, i.e. application of this algorithmic system on the Grid. By the end of 2006 a new approach towards algorithmic systems applications was invented by CIR, the “Grid Library Applications” approach, and will be one of the important development issues inside CIR during 2007.

During 2006 the EU FP6 SEE-GRID project, in which RBI/CIR played an important part, was successfully reviewed and finished. RBI/CIR organized, during the SEE-GRID and now during the SEE-GRID-2 project, the collection, analysis and publication of Present and Future Grid Applications, which enables scientists from a myriad of fields to more easily, find Applications covering their interests. The resulting project Deliverables were sent, on their request, to the EGEE-II project, and recently EGEE-II started a similar effort.

The SEE-GRID project was immediately followed by the EU FP6 SEE-GRID-2 project with a concomitant doubling of the budget. The expertise of CIC in the area of Applications and Application development was recognized in the SEE-GRID-2 project, so that RBI/CIR was given to lead the WP4 (Applications) work package, sharing certain re-

sponsibilities with Turkish partner.

As a third party on the SEE-GRID-2 project CIR included the Faculty of Graphical Arts, Zagreb, university institution which is very important in the general direction of CIR towards Scientific Visualisation.

RBI/CIR, together with the Faculty of Graphical Arts, is working on a Grid Application called VPPR (Visual Parallel Processing and Rendering). The first version of this Application was already used in educational activities for the representation of models of the Tesla multiphase motors.

### Information system development and service

Information Systems Department provides all equipment, tools and other software components to Services department as well as R&D department.

In year 2006 we implemented HORDE Webmail interface, AAI@EdU.Hr system for authentication and authorization, part of LDAP synchronization with human resources database, user interface for password management on LDAP directory. All of these innovations are open source or our own software that are modified to meet our needs.





Figure 2. European Research Area, EGEE member nodes

Regarding network projects we made project for Local Area Network Infrastructure for laboratory in Šibenik and implementation of this project will take part in 2007. In IV wing we coordinated implementation of new network infrastructure as well as new network and telephony closet in the same building. In that part of building it is possible to use same socket for computer and for telephone, but not at the same time.

HORDE Webmail interface (<http://web-mail.irb.hr>) is a new interface for reading mail over web browser. In addition it has built in mail filters, address book, calendar, to do list, notes and weather forecast so it can be replacement for Personal Information Manager (PIM) such as Outlook. In mail functionalities it supports directories so user can sort his mail messages automatically (via built in filters) or manually by putting mail messages in appropriate folder.

AAI@EdU.Hr (<http://www.aai.edu.hr>) is system provided by CARNet, it uses LDAP and RADIUS protocol to authenticate and authorize users among Croatian academic society. Benefits of this system are that now every scientist from our institution can use VIP Mobile Broadband cards to access Internet, all students can access Internet in students dormitory and all other services that are AAI compliant.

We managed to establish semi automated process for database synchronization between Human resources database and our LDAP directory. This improvement was necessary for our intention of interoperability between all departments in Institute to get data from their source, not from second or third level of synchronization. Another aspect is security because now we know who is employee and who is not and to whom we can open electronic identity and to whom not. We sent our proposal of rulebook for electronic identities to our management so we can have legal cover for management of electronic identities.

User interface for password management on LDAP directory is a home made solution for managing LDAP passwords. Every user can log in to this interface (<http://imenik.irb.hr>) and change password. In the future users will be able to manage all their data such as room number, telephone number and other stuff related to them.

Besides the new implementations, we manage whole network and Server Park as well as providing new employees with electronic identity, e-mail address, network connection and other related services.

## SERVICE AND MAINTENANCE DEPARTMENT

Our helpdesk is continuing it's usage of OTRS Ticketing System which has shown itself as indispensable tool for our everyday operations. Printing and TCR services continue to function without any interruptions.

IRB webpage is showing steady increase both in unique visitors as well as in number of visits. Web site is being monitored by our

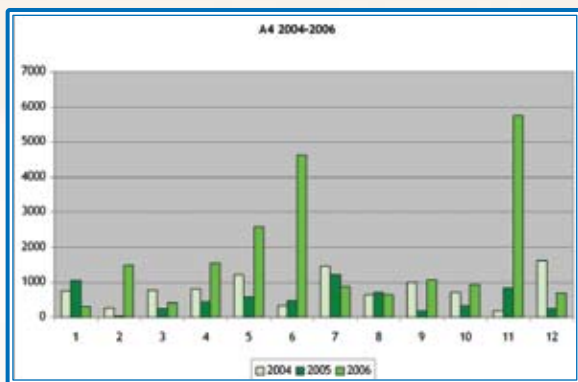


Figure 3. Total number of A4 printouts by month from year 2004 to year 2006.

Total number of A4 printouts for year 2005 was down 35% in comparison to the year 2004 while year 2006 saw 228% percent increase in comparison to the year 2005.

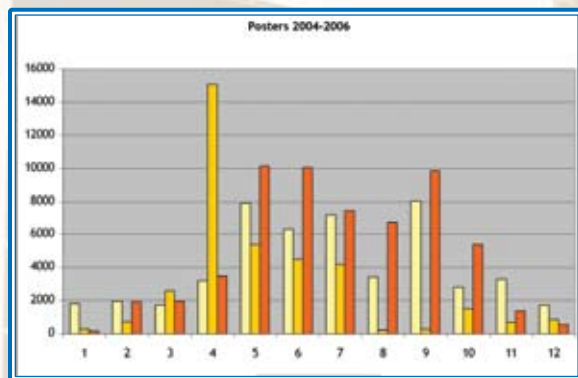


Figure 4. Total length of printed posters (in cm) by month from year 2004 to 2006.

Total length of printed posters (in cm) for year 2005 was down 26% in comparison to the year 2004 while year 2006 saw 62% percent increase in comparison to the year 2005.

own local open-source AWStats system and Google Analytics. Overall it's business as usual in Services and Maintenance department.

## PROMOTIONAL ACTIVITIES

- During the Marie Curie Workshop in Zagreb the presentation of the Tesla Continuum film and the film itself were given to a lot of high ranking educational, academic and political figures, including inter alias the European Commissioner for Science & Research, mr. Janez Potočnik.
- During the opening ceremony of the Institute for Informatics Innovations in Sveti Križ Začretje a promotional animated presentation about CRO GRID and EU Grid initiatives was shown to the Prime Minister of the Republic of Croatia, mr. Ivo Sanader, and the members of the Croatian Government.
- The Second GridVision Teleconferencing Christmas Party was organised by RBI/CIR. This, GridVision Christmas Party, which is starting to be a Christmas tradition for Grid developers all over Europe, connected many European institutions. The Party was co-hosted by CERN, and was announced as an EGEE-II NA2 (Dissemination) event.

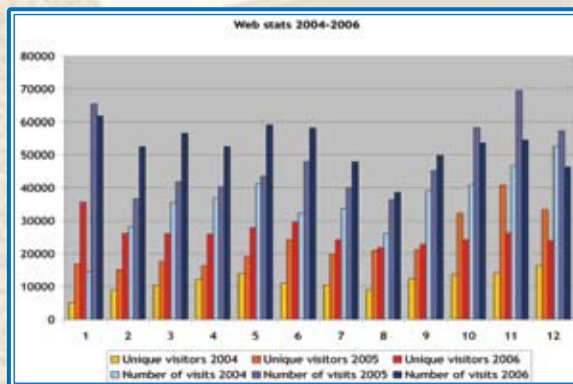


Figure 5. Web server statistics

Total number of visits for the year 2004 was 427.480, in the year 2005 there were 581.906 visits (36% increase) and in the year 2006 there were 630.974 visits (8% increase).



## TOP ACHIEVEMENTS OR HIGHLIGHTS IN 2006

### Development of new technology and equipment

- Finished the EU FP6 SEE GRID project with excellent review.
- Very successful end of CRO GRID project.

### Infrastructure support improvements

- HP blade cluster installation and EGEE Grid Integration.
- Implementation of P-Grade Grid portal.

## EDUCATIONAL ACTIVITIES

- CIR provides 5 undergraduate and 3 graduate courses at Faculty of Electrical Engineering and computing and Faculty of Graphical Arts at the University of Zagreb
- Attendance at the International Grid Summer School on Grid Computing, Budapest, Hungary 3 - 8 July 2006.
- Workshop on Parallel programming and Cluster Technologies, MIPRO Opatija may 2006.
- For the Grid dissemination, CIR continued the updating and maintenance of the Grid-Vision site (<http://gridvision.irb.hr/>), where a myriad of information and links are presented, together with a growing repository of short to medium size films on CIR, Grids in general, EGEE-II and SEE-GRID 2.
- 2006 was the International Year of Nikola Tesla. Together with the Nikola Tesla Association from Zagreb, RBI/CIC co-produced a complex educational animated film "Tesla Continuum" (can be viewed and downloaded from <http://gridvision.irb.hr/>). The film is intended to show the development from the analogue technology grids, as, mostly, invented by Tesla, towards the present day digital technology grids (i.e. computer Grid...). The film consists of two types of animation – analogue (hand drawn) and digital (computer modelled). The music in the film represents the same ideas through the use of different analogue and digital sounding "instruments". The film got a

"Best Presentation Award" at the Marie Curie Workshop in Zagreb. The film was partly co-financed by the Parliament of the Republic of Croatia and Ericsson Nikola Tesla company Zagreb.

- Parallel to the abovementioned, as a part of the Analogue/Digital Grid project, an educational Blog was established, with the attendance of many students and experts in the field (see: <http://ad-grid.irb.hr/>).
- At the Mostar University Faculty of Mechanical Engineering and Computing (<http://www.fsr.ba/>), in cooperation with the SEE-GRID-2 project CIR organized a Training/Workshop on Parallel Programming, Cluster Technologies and Grid Usage.
- Together with the Faculty of Graphical Arts, Zagreb (<http://www.grf.hr/>) CIR developed a Web based interface Application for the representation of 3D models of the Tesla multi-phase motors. Users can specify motor parameters, and will see the 3D model in full "operation".

## 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 ([www.sailing.hr](http://www.sailing.hr)).

## SCOPE OF THE PROJECTS

### Applied scientific project

1. Scientific Visualisation Methods (2007-2010), Karolj Skala

### Technological projects

1. CRO GRID Infrastructure, STRIP, Karolj Skala
2. CRO GRID Applications, STRIP, Karolj Skala

## International projects

1. Grid enabled Infrastructure Development, SEE GRID, EU F6, Con. No. 002356, Karolj Skala
2. Enabling Grids for E-science-II (EGEE-II), EU F6, Con. No. 031688, Karolj Skala
3. South Eastern European GRid-enabled infrastructure Development (2 SEE GRID 2) EU FP6, Con. No. 031775, Karolj Skala

## SOFTWARE PRODUCTS

- ThermoWEB-Remote control and temperature measurement over WEB
- PARF, Parallel Random Forest Algorithm Gridification,.

## ESTABLISHMENT OF NEW INSTITUTIONS

- CIR was the moving factor of the establishment of cooperation between the Ruđer Bošković Institute and the Institute for Informatics Innovations, which resulted in the founding of the commercially oriented project „Kernel for Intelligent Systems and Networks“ (Croatian: "Jezgra za inteligentne sustave i mreže")
- Initiatives between RBI and VIDi to establish the eNovation Award

## COLLABORATION WITH OTHER INSTITUTIONS

- CERN, Geneva, Switzerland
- Štefan Jožef Institute, Ljubljana, Slovenia
- Hungarian Academy of Science Institute SZ-TAKI, Budapest, Hungary
- EU FP6 Consortium member of SEE-GRID-1 and 2
- CRO-GRID Consortium member
- EGEE-II CRO-GRID JRU Consortium member
- Contract for collaboration in GRID technology, Ericsson Nikola Tesla, Zagreb
- Memorandum of Joint ICT development, SRCE, Zagreb
- Faculty of Electrical Engineering and Computing Zagreb
- Mentor Graphics/Wedasoft, Vienna, Austria
- Clinic for tumours, Zagreb, Hrvatska

## SELECTED PUBLICATIONS

1. Kolarić D, Skala K, Dubravić A: ThermoWEB-remote control and measurement of temperature over the WEB, Period Biol 2006:108:631.
2. Topić G, Skala K, Kukulj V, Stevanović R, Šojat Z, Ranec V: From Local Networks to Global Grids: Marie Curie Workshop, Zagreb & Belgrade, 7-11.10.2006.



## ORGANIZATION OF THE CENTRE

Head: Dražen Vikić-Topić  
Substitute: Željko Marinić

The Center for NMR consists of the following groups:

- ⇒ NMR group,  
Dražen Vikić-Topić  
(Substitute: Željko Marinić)
- ⇒ Glass group,  
Andrea Moguš-Milanković



port the experimental measurements. Part of the investigation is focused on the natural compounds and photochemistry products. The second part involves research on the structural and electrical processes in various types of glasses, glass-ceramics and ceramics. In addition, the Centre contributes to undergraduate and graduate studies at the Universities of Zagreb, Osijek and Rijeka. The research includes the application of the following equipment at RBI: Bruker Avance 300 and 600 MHz NMR spectrometers and Alpha AN Impedance Analyzer, Novocontrol Technologies. The subsidiary of NMR Centre located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb is using Varian Gemini 300 MHz NMR spectrometer.

## OVERVIEW OF THE CENTRE

The Centre for Nuclear Magnetic Resonance (NMR), the only academic NMR facility in Croatia, was founded in November 2003 as an independent unit of the Ruđer Bošković Institute. The Centre performs scientific research and service for the scientists and researchers from the Ruđer Bošković Institute (RBI) and from the Universities of Zagreb, Rijeka, Split and Osijek. The Centre provides educational and professional support for the researchers from governmental institutions and pharmaceutical industry. Research work at the NMR Centre includes different topics in organic, inorganic, bioorganic, pharmaceutical chemistry and biotechnology. Theoretical calculations of molecular structures and NMR spectral parameters are carried out in order to sup-

## TOP ACHIEVEMENTS

### Protein-lipid interaction

The experimental evidence of a direct non-covalent interaction of the protein part with the lipid matrix was provided. The approach was based on  $^1\text{H}$  NMR (600 MHz) spectroscopy and thiol-specific spin labelling of the protein (apoB). It was shown that the

$^1\text{H}$  spectral lines assigned to the methyl head groups of phosphatidylcholine and sphingomyelin in low density lipoprotein exhibit line broadening while otherwise free thiol groups of apoB are covalently modified by methane-thiosulfonate spin label. The effect is similar in the presence of a water soluble paramagnetic compound. These results indicate that fragments of apoB, which are part of the receptor binding region, are directly in contact with the solvated phospholipid head groups of the lipid matrix. (Kveder M et al., Chem Phys Lipids 2006: 141: 225)

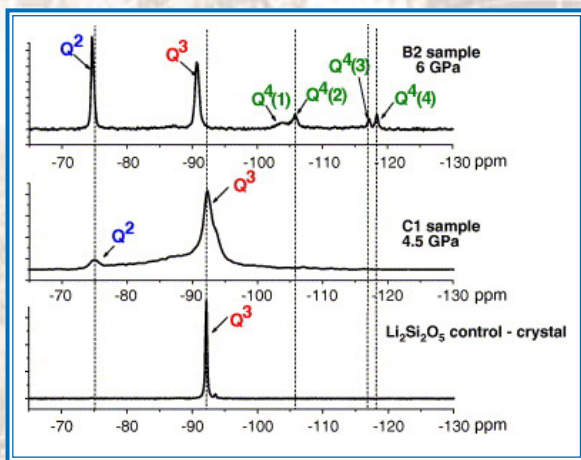


Figure 1. NMR spectra for samples of lithium disilicate glass that crystallized at 4.5 GPa ( $T_{TC}=608^\circ\text{C}$  for 20 min) and at 6 GPa ( $T_{TC}=753^\circ\text{C}$  for 60 min). NMR spectra of crystalline  $\text{Li}_2\text{Si}_2\text{O}_5$  is shown for comparison.

### Crystallization of glasses under pressure

The effect of pressure on the viscosity and structure of silicate melts has been, for the last decade, an area of great interest to geologists and material scientists. It was found that a pressure of above 4.5 GPa is adequate to introduce significant structural changes in lithium disilicate glasses, while even below the melting temperature of  $750^\circ\text{C}$ , 6 GPa pressure is sufficient to form a previously unknown denser crystalline phase. The structural analysis of these transformations sug-

gests that the density of the novel crystalline form of lithium disilicate is higher because the applied pressure reduces the glass free molar volume by deforming the Si-O-Si bonds between neighbouring  $\text{SiO}_4$  tetrahedral. This new crystalline phase represents a new form of lithium metasilicate solid solution. (Fuss T et al., J Non-Cryst Solids 2006: 352: 4101).

## PROJECTS

### Projects supported by the Ministry of Science, Education and Sports

1. Nuclear Magnetic Resonance and Calculations of Bioorganic Molecules, Dejan Plavšić (Dražen Vikić-Topić)
2. Structure and electrical relaxation in glasses and glass-ceramics, Andrea Moguš-Milanković

### International and collaborative projects

1. NMR Study and Modelling of Pharmacologically Applicable Peptides, Željko Marinić (Dražen Vikić-Topić), bilateral collaboration with Slovenia
2. NMR Methods for Structural Analysis of Peptidoconjugates, Vilko Smrečki (Dražen Vikić-Topić), bilateral collaboration with Austria

### Other projects

1. Electrical polarization of bioactive glasses, Andrea Moguš-Milanković, The Foundation of the Croatian Academy of Sciences and Arts

### Contracts with industry

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



## International collaborations

1. Delbert E. Day, University of Missouri-Rolla, MRC, Rolla, MO, USA
2. Nenad Juranić, Mayo Clinic and Foundation, Rochester, MN, USA
3. Norbert Mueller, Institute of Chemistry, Johannes Kepler University, Linz, Austria
4. Marjana Novič, National Institute of Chemistry, Ljubljana, Slovenia
5. Ljupče Pejov, Faculty of Natural Sciences and Mathematics, Skopje, Macedonia
6. Janez Plavec, National Institute of Chemistry, Ljubljana, Slovenia
7. Milan Randić, National Institute of Chemistry, Ljubljana, Slovenia
8. Signo T. Reis, Energy and Nuclear Research Institute, Pinheiros, Sao Paulo, Brazil
9. Nicolay Sergeev, Department of Chemistry, Moscow State University, Moscow, Russia
10. Vladimír Sklenar, Faculty of Science, Masaryk University, Brno, Czech Republic
11. Jure Zupan, National Institute of Chemistry, Ljubljana, Slovenia
2. Smrečki V, Shen L, Ji H-F, Sivanandam VN, Müller N. CSA Tensor of Peptide Backbone Atoms. Dependence on Conformation and Hydrogen Bonding. The Fifth International DU NMR Course and Conference, Mali Ston, Croatia, November 04, 2006.
3. Vikić-Topić D. Croatia Towards the Knowledge-Based Society. The Fifth International DU NMR Course and Conference, Mali Ston, Croatia, November 04, 2006.
4. Vukičević D, Vikić-Topić D, Graovac A. On Application of Directed Graphs to NMR Spectroscopy. The Fifth International DU NMR Course and Conference, Mali Ston, Croatia, November 03, 2006.
5. Moguš-Milanković, A. Electrical Relaxation in Phosphate Glasses, University of Muenster, Institute für Physikalische Chemie, Muenster, Germany, September 07, 2006.



Figure 2. Alpha AN Impedance Analyzer, Novocontrol

## INVITED LECTURES AT INTERNATIONAL CONFERENCES

1. Jadrijević-Mladar Takač M, Vikić-Topić D. NMR and Pharmacy - Long-Range Friends. Regulatory, Pharmaceutical Research and Biomedical Aspects. The Fifth International DU NMR Course and Conference, Mali Ston, Croatia, November 03, 2006.

## SELECTED ORGANIZED CONFERENCES AND COURSES

1. The 21<sup>st</sup> Dubrovnik International Course & Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Dubrovnik (IUC), Croatia, July 19-24, 2006.
2. The 5<sup>th</sup> International DU NMR Course and Conference, Mali Ston, Croatia, November 02-05, 2006.

## EDUCATIONAL ACTIVITIES

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. Modelling 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.
6. Investigation and Application of Inorganic Materials, Graduate Course at University of Zagreb, School of Sciences, Chemistry, Andrea Moguš-Milanković.
7. Bioactive Materials: Investigation and Application in Medicine, Graduate Course at University of Rijeka, School of Medicine, Andrea Moguš-Milanković.
8. Biomaterials, Graduate Course at Ruđer Bošković Institute, University of Osijek, University of Dubrovnik, Andrea Moguš-Milanković
9. Dental Materials, Undergraduate Course at University of Zagreb, School of Dentistry, Andrea Moguš-Milanković.

## AWARDS

Dejan Plavšić: The First International Award Latium between Europe and the Mediterranean for Medicine, Physics, or Chemistry. Rome, 2006.

## SELECTED PUBLICATIONS

1. Kveder M, Marinić Ž, Kriško A, Vikić-Topić D, Pifat G: Lipid-Protein Interactions in Human Plasma LDL Evidenced by Magnetic Resonance. *Chem Phys Lipids* 2006: 141: 225.
2. Landek G, Vinković M, Kontrec D, Vinković V: Influence of Mobile Phase and Temperature on Separation of 1,1'-Binaphthyl-2,2'-Diol Enantiomers with Brush Type Chiral Stationary Phases Derived from L-Leucine. *Chromatographia* 2006: 64: 469.
3. Pilepić V, Jakobušić C, Vikić-Topić D, Uršić S: Evidence for proton transfer from carbon to chloride ion in solution. *Tetrahedron Lett* 2006: 47: 371.
4. Popović Z, Pavlović G, Vinković M, Vikić-Topić D, Rajić Linarić M: Coordination modes of 3-hydroxypicolinic acid (OH-picH): synthesis and characterization of cadmium(II) complexes. Crystal and molecular structures of  $[\text{CdX}(\text{OH-pic})(\text{OH-picH})(\text{H}_2\text{O})]_2$ ,  $\text{X}=\text{Cl}^-, \text{Br}^-$ . *Polyhedron* 2006: 25: 2353.
5. Randić M, Zupan J, Vikić-Topić D, Plavšić D: Novel Unexpected Use of a Graphical Representation of DNA: Graphical Alignment of DNA Sequences. *Chem Phys Lett* 2006: 431: 375.
6. Škorić I, Flegar I, Marinić Ž, Šindler-Kulyk M: Synthesis of the Novel Conjugated  $\omega, \omega'$ -Diaryl/Heteroaryl Hexatriene System with the Central Double Bond in a Heteroaromatic Ring: Photochemical Transformations of 2, 3-Divinylfuran Derivatives. *Tetrahedron* 2006: 62: 7396.
7. Basarić N, Marinić Ž, Šindler-Kulyk M: Photochemistry of o-Pyrrolylstilbenes and Formation of Spiro-2H-pyrroles and their Rearrangement to Dihydroindoles. *J Org Chem* 2006: 71: 9382.
8. Bengisu M, Brow RK, Yılmaz E, Moguš-Milanković A, Reis ST: Aluminoborate and aluminoborosilicate glasses with high chemical durability and the effect of  $\text{P}_2\text{O}_5$  additions on the properties. *J Non-Cryst Solids* 2006: 352: 3668.
9. Fuss T, Moguš-Milanković A, Ray CS, Leshner CE, Youngman R, Day DE: Ex-situ XRD, TEM, IR, Raman and NMR Spectroscopy of crystallization of lithium disilicate glass at high pressure, *J Non-Cryst Solids* 2006: 352: 4101.



Head of Library: Jadranka Stojanovski

## OVERVIEW OF LIBRARY ACTIVITIES

The RBI Library continues to be an essential component of RBI's outstanding research and education mission. The combination of traditional collections and licensed digital resources, accessible via innovative interfaces, and supported by responsive services, provides RBI with a Library that is worthy of this high-class institution. Through our current membership in national CARNET consortia and projects, we are working hard to enhance the Library collections and services, as well as raise our national visibility.

## GOALS AND OBJECTIVES

Our main goal still remains to bring collections and services to the researchers and students "where they work". The Library continues to exist both as a physical and a virtual entity. In 2006 the average number of visits of our library web site is more than 3000 daily. We try to provide services to the Institute in support of RBI's information needs by integrating traditional and digital resources and services, to build and preserve the collections according to a rational collection policy, to organize the collection for effective use, to foster a productive and collegial work environment in which staff have the flexibility and support to achieve their assigned responsibilities, to promote more efficient use



of existing Library resources, and finally, to add new resources to advance the Library's mission.

The main objectives are focused on the development of a strategic plan for institutional repository implementation, the reviewing of trends in technology as well as services and resources so as to provide useful services and support for users. We are also working on the implementation of the new Library Management System, which involves anticipation and response to changes in scholarly communication based on opportunities in electronic publishing.

## SPACE

The limitation of the Libraries' physical space continues to present operational challenges to the Libraries' staff, as well as barriers to researchers in their use of the Library collections, which, despite the fact that journals, handbooks, and databases are increasingly available on the network, are still heavily used. At a time when many thought that electronic publishing would make print obsolete, we are faced with ongoing and increasing difficulties in housing our print collection.

## COLLECTIONS

### Digital collection

The journal acquisition model in 2006 was turned completely toward main world publishers as Elsevier, Springer, Wiley, Blackwell etc., subscribed on the national consortia level directly by the Ministry of Science, Education and Sports. Although more than 12000 e-journals were subscribed, we realized discontinuity in subscription for some very important titles published by "smaller" publishers. The access to the e-journal collection, as to the relevant bibliographic and full-text databases, was realised through the Centre for online databases (<http://www.online-baze.hr>) and newly developed Library portal to e-journals Pero (<http://knjiznica.irb.hr/pero>). RBI researchers can now use over 60 databases, 20000 e-journals and 42 e-books over the Internet.

### Printed collection

While the electronic resources account for most of our time and attention, even the reduced numbers of print publications remain an important part of our collection and will continue to do so well into the future. In 2006, we subscribed only 60 printed jour-

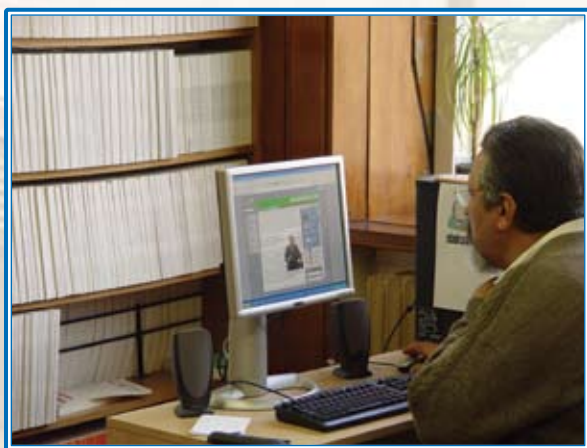


Figure 1. The majority of the resources are available online.

nals. After comprehensive book revision, made during the autumn of 2006, the book collection amounts to 21000 volumes, 200 of which were newly acquired in 2006.

### Interlibrary loan

RBI Library collection, besides being a tool that makes research and scholarship possible at RBI, serves a larger purpose. Library collections represent accumulated knowledge which is important for the research at RBI, but also serve a global scholarly community. The RBI Library has a well-established interlibrary loan service with Croatian and foreign libraries. In 2006 it fulfilled 870 requests for documents made by RBI staff, and over 700 requests from other libraries. The majority of our interlibrary loan requests now come to us online. Through cooperation with numerous libraries we build and extensive shared collection of greater depth than any of the libraries could build alone.

## SERVICES

The RBI Library web site is the place where we incorporate our digital collections and services. The Library web site is main access point to the online catalogue and networked resources. In 2006 the Library web site received over 90,000 visits in an average month. The virtual library serves the same diverse population as the physical library, so we organize it to accommodate multiple levels of researcher's demands. The Library web site is maintained and enhanced by Library staff for the benefit of the entire research community.

The Library is working systematically on an extension of the network services made available to 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 al-



lowing much of the basic library staff assistance to be given indirectly. This assistance included:

- SEND - Interlibrary Loan service (<http://send.irb.hr>)
- CROSBI – Croatian Scientific Bibliography (<http://bib.irb.hr> or <http://crosbi.szi.hr>)
- Who's Who in Croatian Science (<http://tkojetko.irb.hr>)
- CMS for web sites of Croatian academic and research libraries (<http://knjiznice.szi.hr>)
- Centre for online databases (<http://www.online-baze.hr>).

## **RBI INSTITUTIONAL REPOSITORY**

Research libraries in Europe and US are beginning the development of Institutional Repositories where their faculty can store and make accessible the results of their research and their teaching materials. These repositories offer faculty a permanent archive for their digital material and a consistent means of exposing it to the world of scholarship. As a part of RBI institutional repository we will also build multimedia archives which will focus on preserving both the history of the Ruđer Bošković Institute and also those materials that are unique and rare.

If properly constructed, this virtual space could be used as a showcase for our research accomplishments. It could also afford a way of enhancing our outreach to the general population, and of promoting our open access values, and public service role.

The institutional repository involves the creation of virtual knowledge spaces, outside commercial publishing, within the RBI, that will be open access, and directly managed and perpetually archived by the librarians themselves.

Several such repositories have been created by leading research institutions in Europe and US, such as CERN and MIT. In 2006 we developed a prototype for such an Institutional Repository at RBI.

## **NEW LIBRARY MANAGEMENT SYSTEM**

In 2006 the new Library Management System was evaluated and selected by Croatian National and University Library for all Croatian higher education and research libraries. The Voyager system was elected to support library functions such as acquisition, cataloguing, and interlibrary loan. Implementation of Voyager will permit the RBI Library to utilize state-of-the art technology for delivering services. During 2007 our outmoded, in-house software which had served the Library well for last twenty years will be replaced during an intensive year of training and implementation.

## **DIGITAL LIBRARY STANDARDS**

Staff members of the RBI Library are also engaged in defining and implementing new international standards which will be required to take the digital library and preservation development agenda forward in the future. These include standards for metadata and content sharing as well as standards for creating infrastructure to support distributed digital preservation.

## **TEACHING**

### **Graduate level**

Library staff members are involved in teaching at University J. J. Strossmayer in Osijek.

## KEKS training

In the process of helping library users formulate research strategies, identify information sources, and discuss methods of accessing resources, librarians educate those they assist. The librarian's goal is to show library users how to become as self-sufficient as possible to ensure that intellectual pursuit and creativity are not frustrated. Our librarians offer short training and workshops on user's sites.

## AWARDS

Jadranka Stojanovski, Kukuljevićeva povelja, 2006.

## TOP ACHIEVEMENTS PERO

We developed the new portal for electronic resources PERO for searching the content of over 20000 commercial and freely available full-text e-journals, selected for relevance and quality.



Figure 2. Portal for e-journals developed at RBI Library.

## CROATIAN SCIENTIFIC PORTAL

With the Croatian Scientific Portal we encompass all existing and new databases about researchers, their scientific output and research projects, providing single access point to all relevant data about science in Croatia.



Figure 3. Croatian Scientific Portal – the main access point for information about research in Croatia.

## SELECTED LECTURES

1. Vodopijevac A: Open code CMS's. 6. Seminar za knjižnice visokih učilišta i znanstvene knjižnice, Zagreb, March 03-04, 2006.
2. Vodopijevac A: Digital repositories of the scientific information. CUC2006, 8. CARNetova korisnička konferencija, Dubrovnik, September 20-22, 2006.
3. Macan B; Vodopijevac A, Grozdanić M: Institutional repository at Ruđer Bošković Institute. Proc. of the conference LIDA 2006: Libraries in the digital age held in Dubrovnik and Mljet, Croatia, May 29-June 02, 2006. / Aparac-Jelušić, Tatjana ; Borgman, Christine L. ; Saračević, Tefko (eds.). Osijek : Department of Information Sciences, University J.J. Strossmayer, Osijek, 2006. 122-123



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1. Open Waters - Open Sources: proceedings of 11th Biennial Conference of the European Association of Aquatic Sciences Libraries and Information Centres (EURASLIC), editors Sofija Konjević, Marina Mayer. Zagreb, Ruđer Bošković Institute, 2006
2. Pažur I: Models of the organisation and access to the e-journals collections in Croatian scientific libraries. Vjesnik bibliotekara Hrvatske. god. 49 (2006) 10.
3. Mayer M: Databases of the European commission for chemists. Kemija u industriji. 55 (2006) 106.
4. Mayer M: E-journal portal Open J-Gate. Kemija u industriji. 55 (2006) 382.
5. Pikić A: Alternative libraries in the city of Zagreb. Vjesnik bibliotekara Hrvatske. god. 49 (2006) 58.
6. Stojanovski J. Wissenschaftliche Informationen aus einer Hand - Erfahrungen aus Kroatien. GMS Med Bibl Inf 2006; 6:Doc08 (20060531).
7. Stojanovski J, Martek A: Croatian Scientific Information System – a good example of the efficient cooperation. Partnerships in the special and high education libraries.: Zbornik radova 7. Dani specijalnih i visokoškolskih knjižnica (Pilaš I, Martek A (eds). Zagreb: Hrvatsko knjižničarsko društvo, 2006: 131.
8. Toth T, Konjević S: Water: open access information sources. Open Waters - Open Sources: proceedings of 11th Biennial Conference of the European Association of Aquatic Sciences Libraries and Information Centers (EURASLIC) (Konjević S, Mayer M (eds). Zagreb, Institut Ruđer Bošković, 2006: 181.
9. Vodopijevac A: City of the Sun, Open Access and Institutional Repositories. Kemija u industriji. 55 (2006) 342.

## CONFERENCE ORGANIZATION

The Croatian academic and special libraries conference of 2006 entitles “Open as...library: Open code and open access in Croatian libraries?” was organized by the Institute's Library, Croatian Academic and Research Network CAR-Net, Faculty of philosophy and Faculty of Science (Department of Physics and Department of Mathematics) at the Faculty of Science, University of Zagreb, Zagreb, from 03.-04.03.2006.



Figure 4. Librarian's 2006 conference with open access as a main topic.

## IT PROJECTS

1. Croatian Scientific portal, including
  - Croatian Scientific Bibliography CROSBI, Jadranka Stojanovski
  - Who's Who in Science in Croatia, Jadranka Stojanovski
  - Portal for Croatian scientific journals HRČAK, Jadranka Stojanovski
2. Centre for online databases, Jadranka Stojanovski.









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.