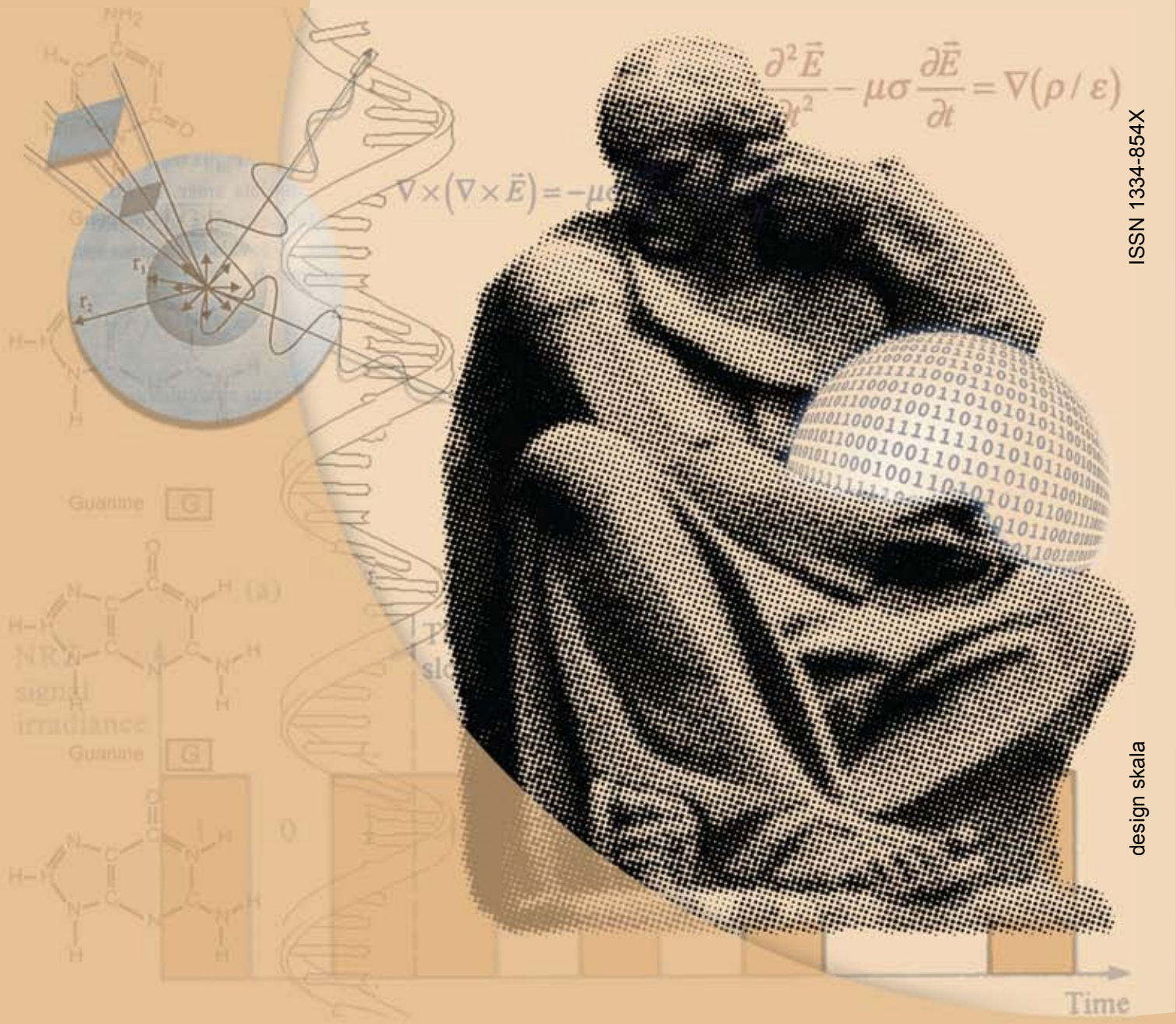

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Ruđer Bošković Institute

Annual Report 2007

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Zagreb, 2008.

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Contents

Dear reader,

Welcome to the 2007 Annual Report of the Ruđer Bošković Institute. The report has been conceived to provide a succinct overview of the most important activities and achievements of Institute's Laboratories and Divisions during the past year. Due to our position as the largest public research institute in natural sciences, biomedicine, marine research and environmental sciences in the country, funded to a large extent by the Croatian Ministry of Science, Education and Sports, our mission is dependent upon the particular needs of our society. Specifically, this involves exemplary performance on three principle fronts: the production of high-quality fundamental research, strong involvement in higher education, and the provision of a leading contribution to the growth of the national economy through production of new technologies based on our intellectual property and expertise. In 2007, we continued to achieve visible results on all three fronts, with a well-balanced mixture of short- and long-term initiatives.

The beginning of the year saw the signing of contracts for new basic research projects with the Ministry of Science, Education and Sport. The research agreed to in these contracts is now underway and the most significant results achieved in 2007 can be found in the pages of this report. In addition to the substantial ongoing provision of undergraduate and graduate courses by our scientists at Higher Education Institutions all across the country, 2007 saw us sign additional agreements of cooperation with Universities in Pula and Rijeka. These agreements are designed to further strengthen our contribution to education in Croatia, particularly in regional centres. We also made several advancements towards the establishment of a sustainable infrastructure designed to fully utilize the Institute's intellectual property in 2007. Much progress was achieved through the ongoing expansion of Ruđer Innovations Ltd., a company established and wholly owned by the Institute, which has been charged with handling the protection of intellectual property and some commercial aspects of the Institute's work.

While a strong involvement in domestic affairs is an important part of our function, it is clear that the current academic climate also calls for an increased external focus. Our scientists are acutely aware of this and have an impressive rate of success in terms of gaining international projects. Naturally, becoming an integral part of the European Research Area is one of our key strategic goals, and our ability to realize it is reflected by our increasing involvement in the 6th and 7th Framework Programmes during 2007. Apart from this, our scientists have also enjoyed noteworthy successes by obtaining projects from other external sources such as IAEA, NATO, COST, as well as numerous bilateral projects with foreign scientific institutions.

To conclude these opening remarks, I take great pleasure in thanking all of the Institute's employees, both scientific and administrative, for their diligent and sustained efforts throughout 2007. The success we enjoy as an Institute stems from the hard work of the individuals that comprise it. I am honoured to be in a position to offer my sincere congratulations to those who enjoyed notable successes this year, but also to everyone for a job well done. Finally, to you the readers of this Annual Report, I would like to thank you on behalf of all of us here for your interest in our activities. I would also like to take this opportunity to inform you that we warmly welcome your opinions and suggestions, even the critical ones, and are always open to incorporating new ideas and collaborative partners into our activities here at the Ruđer Bošković Institute.

Prof. Dr. Mladen Žinić
Director General

Introduction

In 2007, the scientific and administrative staff of the Ruđer Bošković Institute (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 2007, the RBI was visited by in excess of 100 foreign scientists originating from countries all over the world. As well as delivering well-received lectures, the visitors typically engaged in initiation or continuation of scientific collaboration. We were honoured to be able to host four members of our International Scientific Board (ISB) in October this year. Namely, Professor Bogdan Povh, from Heidelberg, enlightened us on the importance of nuclear and elementary physics in the modern day research in October. Professor Fernando Azorin, from Barcelona, explained the epigenetic regulation of centromere identity and function, while Professor Bernd Kaina, from Mainz, educated us on the O6-alkylguanine response, including mechanisms and clinical implications. In early February, the RBI was honoured to host Professor Julius Wess, an esteemed physicist from LMU, München.

We were also very pleased to be able to receive His Excellency Kapil Sibal, the Minister for Science and Technology of the Republic of India and his delegation in February. Our scientific collaboration with India is developing well through active participation of RBI researchers, based on the bilateral agreement on cooperation in science and technology, signed last year.

The participation of RBI scientists in European scientific networks remained one of the Institute's top priorities in 2007. RBI continued active collaborations in different COST actions and succeeded to contract an additional 5 FP6 projects reaching a total number of 19 FP6 projects contracted up to the end of 2007. By the end of the year, several FP7 projects were also being evaluated or negotiated. RBI scientists also took an active role in Management Committees of COST actions. Krešimir Pavelić, head of the RBI's Division of Molecular Medicine was re-elected as a vice president of EMBO and Tarzan Legović, head of the Division of Marine and Environmental Research was again appointed Secretary General of the International Society for Ecological Modelling.

The RBI signed several Memoranda of Understanding in 2007. On the industrial side, agreements were signed with firms such as Shimadzu, Chiyoda Technol Corporation (CTC), and Alkaloid Skopje, as well as a general understanding of cooperation with the scientific research consortium Joanneum Research in Graz and the Jožef Štefan Institute in Ljubljana. In the area of higher education, agreements were reached with the University Jurja Dobrile in Pula and, closer to home, with the University of Zagreb.

An ongoing collaboration between the Division of Materials Physics and the Lipik-Glass company was significantly strengthened in 2007 by the signing of a three year project co-financed by Lipik-Glas and the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia. Similarly, a research and development project focusing on the reliability of programmable logic devices in in-

dustrial embedded systems and financed by the Končar Institute for Electrical Engineering, was signed with the Division of Electronics. This project is mediated through Ruđer Innovations Ltd., the company established by the RBI last year to assist with commercial affairs and intellectual property protection. Within the framework of the TEST program of the Croatian Institute of Technology (HIT), an additional contract was signed in the Division of Experimental Physics for a project concerning the development of a photon detector for applications in security, diagnostics, and analytical methods.

Building on the success of its first year of appearance in 2006, when founded by RBI and VIDI magazine, the E-novation Award attracted more than 30 applications from companies, academic institutions and individuals in 2007. An important aspect of the E-novation Award, proven for a number of last year's Award-winners and participants, was that most of them obtained a significant boost in terms of visibility and credibility of their invention, which resulted in real economic benefits.

The Institute's own scientists were also quite inventive this year. As an example, Ruđer Innovations Ltd. showed a strong presence at the 5th international ARCA exposition of inventions, new ideas, products and technology in September. There they presented three projects from the company Initium Futuri Ltd., three innovative ICT projects, a software package based on the Robin Hood method (developed by RBI scientists), and Ruđer-Medikol Diagnostics Ltd.

OVERVIEW

The RBI 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 581, including 362 researchers, 219 Ph.D. students, the RBI collaborates worldwide with many research institutions and universities.

The RBI consists of twelve divisions, three 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).

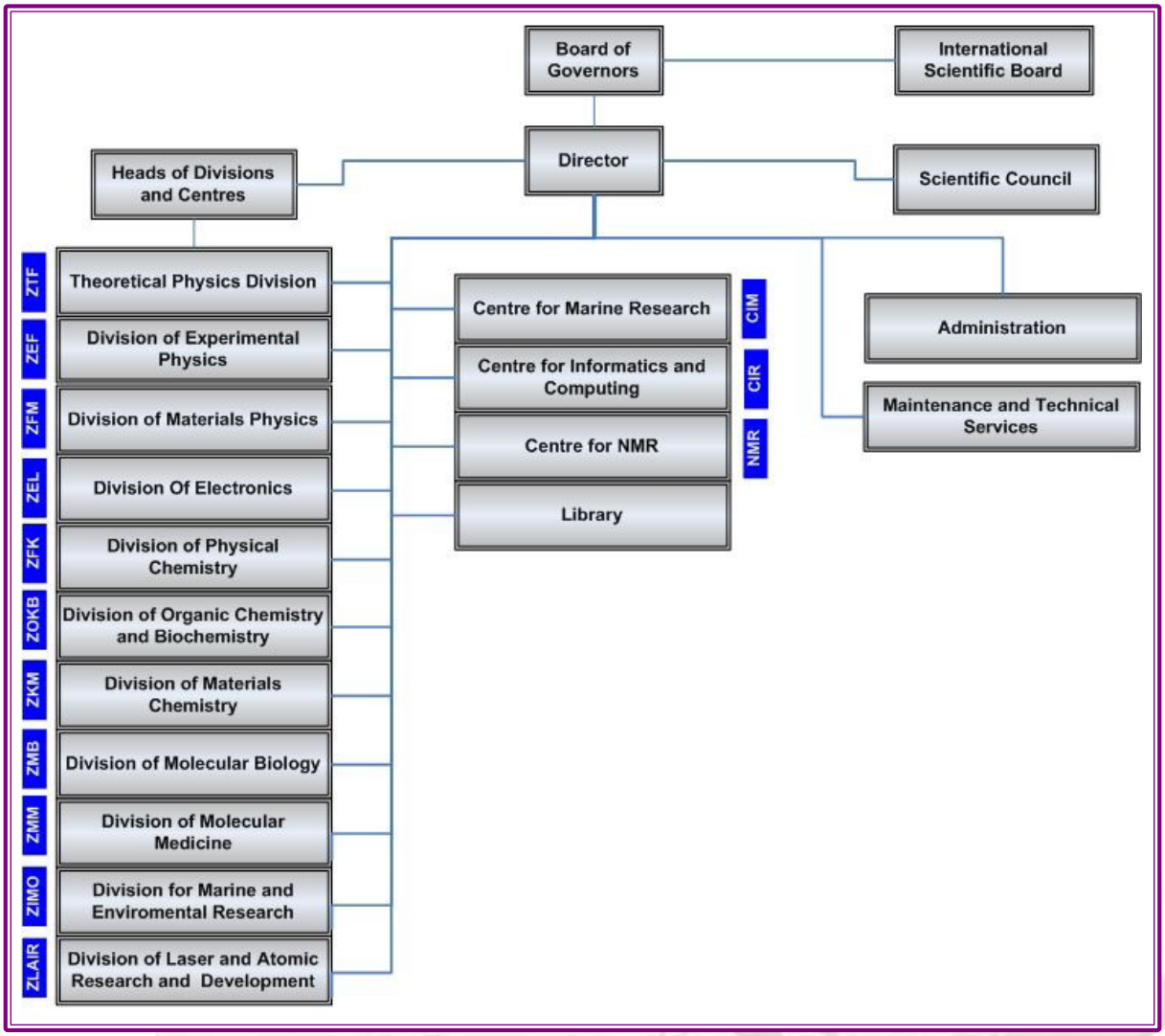

Figure 1. The organizational structure of the RBI

ORGANIZATION OF THE INSTITUTE

Director: Mladen Žinić
Head of the Scientific Council: Maja Osmak (until March); Neven Bilić
Chairman of the Board of Governors: 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
- Robert Blinc, Jožef Štefan Institute, Ljubljana, Slovenia
- Jonathan R. Ellis, CERN, Switzerland
- Anthony R. Peaker, University of Manchester, UK
- Bogdan Povh, MPI für Kernphysik, Heidelberg, Germany
- Roberto D. Peccei, UCLA, Los Angeles, CA, USA
- 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, Jožef Štefan 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 2007 was 450. Among these, 395 were published in journals cited by Current Contents. With less than 6% of the total number of scientists in the country working at the Institute, it is worthy of note that 22% of all Croatian articles in Current Contents journals originated from the RBI. A considerable proportion of these articles were published in high ranking journals. In 2007 the scientists from RBI edited a handbook about the methods in molecular biology, four monographs, and 8 book chapters.

Many important discoveries were made by RBI scientists in 2007. Far too many, in fact, to list here and the reader is referred to the subsequent sections of this report for a more detailed presentation. One study that typifies the type of interdisciplinary research at the Institute involved contributions from scientists working in the Divisions of Molecular Medicine, Organic Chemistry and Biochemistry, Physical Chemistry, and Electronics. This team of researchers investigated the potential anti-tumour ability (including

cell cycle and cell death studies) and structure-activity relationships of various crown ethers and their derivatives. Their findings were published in the Journal of Medicinal Chemistry, a very respectable and high impact periodical in that field. Another discovery that captured a broad public interest in 2007 was the development, in the Division of Molecular Biology, of an innovative approach to understanding the origins of evolutionary novelties in the animal kingdom. This technique, known as genomic phylostratigraphy, involves the analysis of genome sequences to uncover the footprints of important adaptive events in evolution and was presented in Trends in Genetics. The results from this work were also favourably evaluated in the Faculty of 1000 Biology, which is a service designed to systematically highlight and review the most interesting papers published in the biological sciences. On the other end of the spectrum, another collaborative effort, involving the Division of Theoretical Physics and the Division of Organic Chemistry and Biochemistry, resulted in a publication in Physical Review Letters, one of the most respected and widely read journals in Physics. This study involved the theoretical modelling of the electronic structure and transport properties of the polymer polyyne, revealing that compounds of this type are virtually perfect molecular wires and represent good candidates for applications in nanotechnology.

Projects

The RBI has 129 projects in basic research, which are funded by the Ministry of Science, Education and Sport (MZOŠ). In addition, the Institute is involved with 56 international projects (including: 18 bilateral, 19 FP6, 12 IAEA, 5 COST, 1 UKF, 1 NIH, 1 NATO, 1 INTERREG and 1 PHARE), as well as 15 applied and technological projects in cooperation with BICRO and HIT. Also, 32 commercial contracts were signed in Croatia as well as 6 contracts with companies from foreign countries.

Organization of international conferences

As in previous years, the RBI continued to support the organization of numerous international and domestic conferences. For example, 2007 saw the 22nd staging of the Dubrovnik International Course and Conference on the Interfaces among Mathematics and Computer Sciences, otherwise known as MATH-CHEM-COMP, from June 11-16. The 4th International Summer School and European School on Solid State NMR: Solid State NMR for Liquid State NMR Spectroscopists, was held in the same city from September 16-21. Further north, in Optaija, a group of motivated young scientists at the Institute received support from both the European Commission and the Alexander von Humboldt Foundation to hold the 2nd Opatija Meeting on Computational Solutions in the Life Sciences from September 4-9. The 6th European Ecological Modelling Conference was organized by the head of our Division for Marine and Environmental Research and held in Trieste, Italy, from the November 27-30. In Rovinj, a conference entitled Long Time-Series Observations in Coastal Ecosystems: Comparative Analyses of Phytoplankton Dynamics on Regional to Global Scales, organized by the American Geophysical Union, as a Chapman Conference, and the Center for Marine Research, was held from October 8-12. Several other equally noteworthy conferences were organized by scientists from the RBI and further information concerning them can be found in the individual reports of the Divisions involved. In addition to their organizational efforts, RBI scientists also participated in many scientific meetings over the year and a notable RBI presence was apparent at both the Croatian-Austrian scientific days in Graz (November 18-19) and the 2nd Congress of Croatian Scientists, held from May 7-10 in Trogir.

Education

Despite the fact that the RBI is primarily a research institution, our participation in educational activities during 2007 was very strong. Scientists from the Institute contributed 83 courses at the undergraduate level as well as 217 postgraduate courses. Last, but not least, more than 25 young scientists from RBI contributed to seminars and practical exercises at various undergraduate studies. The respective distribution amongst the universities at which they were conducted, as well as by the divisions and centres that contributed the graduate course, are shown in Figures 2-4. In 2007, 22 B.Sc., 32 M.Sc. and Ph.D. theses were completed under the supervision of the Institute's academic staff.

To strengthen the collaboration with regional Universities and increase the contribution in higher education in natural science, the RBI signed agreements of cooperation with the University Juraj Dobrila University in Pula. Shortly after, the preparations for the organization of joint graduate and postgraduate studies in Medicinal Chemistry in collaboration with the University of Rijeka and GlaxoSmithKline Research Centre Zagreb, were begun. A novel PhD study program „Biology of Cancer" was launched in 2007 jointly by the RBI and the Universities of Split, Dubrovnik and Zadar. It is the first national PhD study program with international evaluation and full ECTS accreditation, with Neven Žarković from Division of Molecular Medicine elected for the Vice-chair of the Study Council. In May, the University of Zagreb and the RBI signed agreements of cooperation concerning collaboration in education, scientific research and partnership in international projects, as well as the commercialization of knowledge and the acquisition of valuable new equipment.

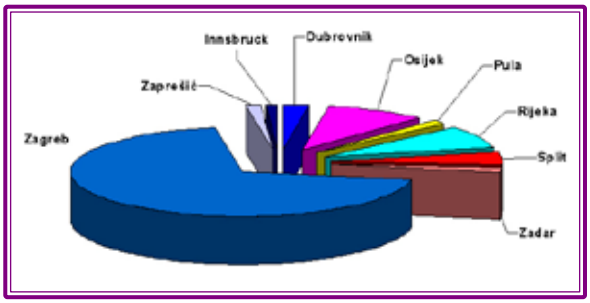

Figure 2. Distribution of the RBI held undergraduate courses among the universities (83)

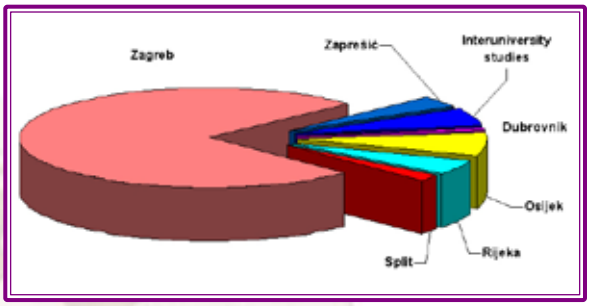

Figure 3. Distribution of the RBI held graduate courses among the universities (217)

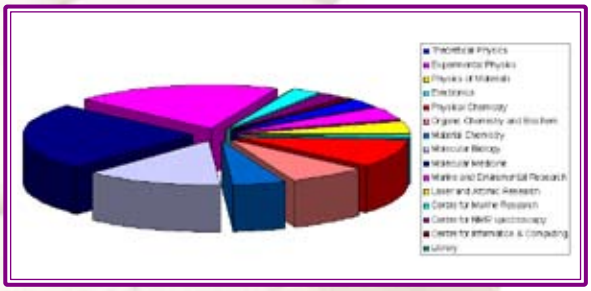

Figure 4. Distribution of the RBI held graduate courses at domicile universities among Divisions and Centres (217)

Intellectual Property

Apart from fundamental research and education, the activities of the RBI also result in various forms of intellectual creations. One important mission of the RBI (also appointed in the Statute) is the protection of intellectual property and its commercialization. In this context, various specific activities have been initiated and realized in this vein over the last few years. For example, the Institute's Commission for intellectual property has been established. The book of regulations on intellectual property was drafted and accepted by both the Board of Governors and the Sci-

entific Council. We have also established a company under the name Ruđer Innovations Ltd. This company, which is wholly owned by the RBI, engages in activities related to protection and commercialization of knowledge arising from the RBI, other academic organizations, companies, and private persons. The establishment of this climate has resulted in heightened interest from the Institute's scientists to protect and commercialize the results of their investigations. As such, many proposals of innovations were received by the Institute's Commission for Intellectual Property over the last few years, the majority of which were submitted in 2007. Presently, the portfolio of the Institute's intellectual property contains 33 innovations in different fields (chemistry, physics, biomedicine, informatics, instrumentation etc.). In accordance with the Master agreement between the RBI and Ruđer Innovations Ltd., the innovations accepted by the Institute's Commission for Intellectual Property are licensed to the Ruđer Innovations Ltd., which carries out the appropriate procedures for protection and commercialization. Presently, 32 innovations have been licensed to Ruđer Innovations Ltd., 21 of them are in various steps of protection, while the remainder are being prepared to be protected.

NEW EQUIPMENT

The Laboratory of Chemical and Biological Crystallography in the Division of Physical Chemistry was the proud recipient of a new X-ray diffractometer this year. The diffractometer (Xcalibur Nova R), from Oxford Diffraction, which was financially supported by the Ministry of Science, Education and Sports, is an X-ray system designed for protein crystallography and applications where a high brilliance copper X-ray source is required. This is the first X-ray equipment in Croatian academic community suitable for a single crystal diffraction of biological macromolecules and this acquisition will enable new interdisciplinary research in the field of (bio)materials and life science. Also, the XRPD RIGAKU HRMP diffractometer arrived to the Centre for Marine Research in Rovinj.

In 2007, the Laboratory for the Synthesis of New Materials, in the Division of Material Chemistry, received an Atomic absorption spectrophotometer Aanalyst-200 (Perkin-Elmer) as well as an Ion Chromatography System, ICS-1000, Dionex Corporation. These acquisitions will greatly facilitate the rapid characterization of new materials.

With the help of an IAEA funded project, a new quadrupole lens was added to the existing quadrupole doublet and a newly designed scattering chamber was installed at the ion microprobe. In such a way, the upgraded quadrupole triplet system provided a significantly better focusing capability of the facility (0.3 x 1 μm). By the installation of additional two quadrupole lenses planned for 2008 under an EU-FP6 project, our quintuplet system will be able to focus ions of up to 25 MeV (ME/Q2) rigidity.

A Iatroscan MK-6, which is thin layer chromatograph measuring samples by means of a Flame Ionization Detector (FID) and a Flame Photometric Detector (FPD), was installed in the Laboratory for Physico-Chemical Separations, in the Division of Marine and Environmental Research. The instrument will greatly enhance the analysis of lipids and the separation of lipid classes from nonpolar lipids such as hydrocarbons and polar phospholipids.

A novel Laboratory for Molecular Biosciences was established in Dubrovnik as a joint research facility of the RBI, University of Dubrovnik and the Dubrovnik General Hospital, to provide research facilities for the joint PhD studies. The Laboratory will further support networking within the B35 Action of COST and affiliated research networks.

Building upon the experience of the CRO-GRID poly-project, the CRO NG (Croatian National Grid Infrastructure) was established during 2007. As part of the important and constant contribution of RBI/CIR to CRO NGI, a new 96-processor computer cluster was installed at RBI for the purpose of furthering scientific research.

Revenue and employees

In 2007, the major share of the financial support for the RBI was provided by the Ministry of Science, Education and Sports. Compared to 2006, this support increased by 15%. The comparison of the finances over the period 2004-2007 (Table 1) shows a gradual increase with the larger steps for 2005/2006 and 2006/2007. Together with the support for a 39% increase in the employment of the PhD students, this clearly shows the strategic orientation of the Ministry toward the development of a knowledge-based society. It should be also noted that the revenues originating from international, industrial and service contracts increased in 2007 by an impressive 59% as the result of enhanced efforts in applications to various international and national calls and a systematic approach toward commercialization of knowledge and skills of the RBI scientists through licensing and research contracts with domestic and foreign industries.

	2004	2005	2006	2007	2007/2006 (%)
Contracts Contracts with Ministry of Science Education and Sports (€)	16.106.768	17.293.472	20.072.940	23.090.639	115
Other contracts (international and industry projects, services etc.) and donations (€)	2.505.920	1.890592	2.311.744	3.671.788	159
total	**18.612.688**	**19.184.064**	**22.384.684**	**26.762.427**	**119**
Employees					
Scientific staff	310	325	317	320	101
post-doctoral students	31	30	40	42	105
PhD students	153	159	158	219	139
technicians	113	127	134	85	63
administration and maintenance	170	174	176	174	99
total	**777**	**815**	**825**	**840**	**102**

Table 1. Comparison of RBI Revenues (€) and employment during 2004-2007.

Publication results of fundamental research projects at RBI

Table 2 shows the projects led by RBI scientists that were ranked among the top 10 in the country, according to the National Bibliography database (web address: http://bib.irb.hr/statistika?sto=p&period=2007). The rank corresponds to the position of a particular project, among the projects that began in 2007, as determined by the number of research articles published in journals indexed in Current Contents (CC) up until March 3rd, 2008. Also included in the Table is the number of CC articles, associated with each project, that were published during 2007. Some limitations of the table are that it does not include aspects such as an average journal impact factor, the number of researchers/students working on the project, and the amount of financial support received by the various projects.

Field of Science - Number of National Projects in the Field	Project Title	Principal Investigator	Rank of the Project in the CROSBI Bibliography on March 3rd, 2008	Number of CC Articles Published in 2007
BIOLOGY - 61	Cell response to cytotoxic agents and resistance development	Maja Osmak	3.	6
	Molecular regulation of plant development	Branka Salopek-Sondi	4.	3
	Genes and genomes: structure, function and evolution	Helena Ćetković	8.	4
PHYSICS - 73	Nuclear structure and reactions: experimental approach	Suzana Szilner	1.	16
	Physic and application of nanostructures and bulk matter	Krešimir Furić	3.	12
	Fundamental interactions in elementary particle physics and cosmology	Branko Guberina	5.	12
	Thin films of novel amorphous or nanostructured materials	Nikola Radić	5.	11
	Basic properties of nanostructures and defects in semiconductors and dielectrics	Branko Pivac	7.	9
	Synergy of nanophases and nanocomposites	Aleksandra Turković	9.	9
	Massive neutrinos and astroparticles: from particle physics to cosmology	Ante Ljubičić	10.	9
GEOSCIENCES - 59	Nature of organic matter, interaction with traces and surfaces in environment	Zlatica Kozarac	3.	8
	Radionuclides and trace elements in environmental systems	Delko Barišić	4.	7
	Interactions of trace metal species in an aquatic environment	Ivanka Pižeta	9.	3
CHEMISTRY - 66	Synthesis and microstructure of metal oxides and oxide glasses	Svetozar Musić	1.	14

	Broensted and Lewis acids and bases in chemistry and biochemistry	Zvonimir Maksić	3.	12
	Self-Assembly in gels and synthesis of functional hybrid materials	Mladen Žinić	5.	8
	Molecular structure and dynamics in systems containing paramagnetic particles	Boris Rakvin	6.	8
	Electroanalytical research on microcrystals and traces of dissolved substances	Milivoj Lovrić	8.	5
	Protein-ligand interactions at atomic level	Marija Luić	10.	7
BIOMEDICAL SCIENCES – Neuroscience- 58	Pharmacogenomics and proteomics of serotonergic and catecholaminergic system	Dorotea Mück-Šeler	1.	10
	Molecular basis and treatment of psychiatric and stress related disorders	Nela Pivac	2.	8
	Serotonergic neurotransmission: genes, proteins and behavior	Branimir Jernej	6.	3
	Stress, GABA-A receptors and mechanisms of action of neuropsychoactive drugs	Danka Peričić	8.	3
	Serotonergic mechanisms in alcoholism	Lipa Čičin-Šain	9.	1
BIOMEDICAL SCIENCES – Oncology - 67	The role of different cell death responses to DNA-damage treatment	Marijeta Kralj	1.	10
	Aberrant DNA methylation in HPV associated lesions	Magdalena Grce	2.	6
	Molecular characteristic of myofibroblasts derived from Dupuytren's contracture	Krešimir Pavelić	3.	5
	Gene therapy of tumors by modulating the molecules of immune system	Jasminka Pavelić	4.	5
	Molecular genetics and pharmacogenetics of gastrointestinal tumors	Sanja Kapitanović	5.	2
BIOMEDICAL SCIENCES - Research of chronic diseases - 73	Obtaining the structures like Langerhans islets from mouse stem cells	Mirko Hadžija	4.	1
BIOTECHNICAL SCIENCES - Agronomy - 132	Subcellular biochemical and phylogenetic diversity of aquatic organisms	Rozelinda Čož-Rakovac	4.	3
TECHNICAL SCIENCES - Electrical engineering	Multispectral data analysis	Ivica Kopriva	9.	1
	Real-life data measurement and characterization	Branka Medved-Rogina	10.	2

TABLE 2: Publication results of RBI fundamental research projects ranked among the top 10 Croatian projects in their respective field.

Theoretical Physics Division

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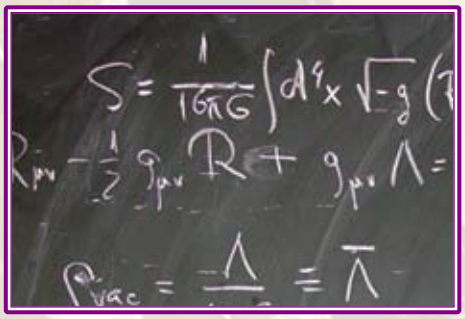

DIVISIONAL ORGANIZATION

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

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 modeling in life science and the application of nonlinear statistical methods in biomedicine. In 2007, the members of the Division continued to be involved in lecturing at the University of Zagreb and a number of students completed their B. Sc., M. Sc. and Ph. D. theses.

TOP ACHIEVEMENTS

Gravitational Trace Anomaly

The quantum trace anomaly has been studied in the context of an infrared effective theory of gravity. By imposing the generalized Bianchi identity, a prediction for the scale dependence of the dark matter and dark energy densities has been obtained in terms of the parameters of the underlying conformal theory. For certain values of the model parameters, the dark energy equation of state and the observed spectral index of the primordial density fluctuations can be simultaneously reproduced (Bilić et al., 2007).

Holographic Dark Energy

The concept of holographic dark energy (DE) constitutes a serious candidate for dark energy of the universe. Some models in which the holographic bound for DE is not saturated for a large portion of the history of the universe have been investigated. It has been demonstrated that a transition between the two eras is always obtained for the IR cutoff in the form of the Hubble scale and the nonsaturated holographic DE. Arguments have been given as to why such a choice is more consistent and to be favoured over the widely accepted saturated form (Guberina et al., 2007).

Strings and Nonlocality

The T-duality of string theory suggests nonlocality manifested as the shortest possible distance. A nonlocal formulation of string theory has been suggested as an alternative that breaks the T-duality at the fundamental level and does not require the shortest possible distance. Instead, the string has an objective shape in spacetime at all length scales and different parts of the string interact in a nonlocal Bohmian manner (Nikolić, 2007).

Waves and solitons in the two-family Calogero model

Soliton solutions in the two-family Calogero model have been analyzed. There are two types of solutions, a one-soliton-antisoliton solution and a wave solution. It was shown that there is no finite number of solitons at finite distances in the limit when the period of wave solutions tends to infinity (Bardek and Meljanac, 2007).

Collective field formulation of the multi-species Calogero model and its duality symmetries

We have studied the collective field formulation of a restricted form of the multispecies Calogero model, in which the three-body interactions are set to zero. We have shown that the resulting collective field theory is invariant under certain duality transformations, which interchange, among other things, particles and antiparticles, and thus generalize the well-known strong-weak coupling duality symmetry of the ordinary Calogero model. We have identified all these dualities, which form an Abelian group, and study their consequences. We also studied the ground state and small fluctuations around it in detail, starting with the two-species model, and then generalizing to an arbitrary number of species (Bardek et al., 2007).

Conduction at the nanoscale

The advances in miniaturization of electronic devices to the nanoscale, utilizing a single molecule as the active region, has recently generated considerable interest both for the fundamental physics involved and for its potential applications. In a search for a molecule with good molecular wire properties we have considered the polyyne, linear chain of carbon atom pairs with alternating single and triple bonds. Based on a non-equilibrium Green functions technique and density functional theory a quantum modelling of the electronic structure and transport under applied bias voltages was carried out. The conductance obtained, which is virtually independent of the length of the molecular chain and an order of magnitude higher than the conductance of other known molecules, put polyynes as almost perfect molecular wires (Crljen and Baranović, 2007).

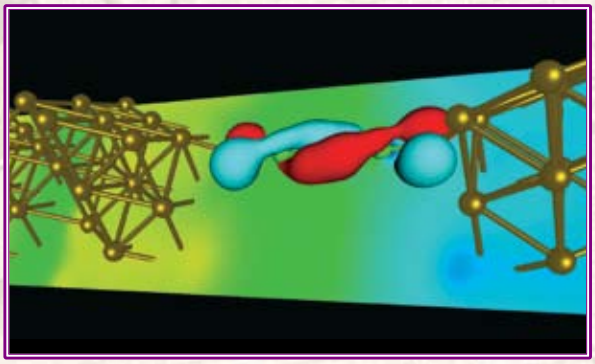

Figure 1: The diyne molecule in contact with gold electrodes and the highest occupied orbital of the molecular projected Hamiltonian at 0.6 V bias voltage. Background colours reflect voltage drop along the structure.

The Robin Hood method: From theory to applications

The Robin Hood method for the numerical solution of boundary problems in electrostatics has seen exciting new developments. The team consisting of three young researchers

has further elaborated the practical aspects of the application to real problems, and an article will be published in the journal Engineering Analysis with Boundary Elements. Their application to the project “From Research to Enterprise” of the Central European Initiative has won a 15.000 Euro award, of which 10.000 Euro was dedicated to the financing of the feasibility study. The resulting ‘Feasibility Study on commercialization for the "Robin Hood" electrostatic field calculation method’ by Professor Günter Koch and co-workers from Vienna, Austria, has shown the potential of the method for commercial applications, and has proposed a commercialization strategy.

EDUCATION

In 2007, the members of the Division continued to be involved in lecturing undergraduate and graduate courses at the University of Zagreb, mostly at the Faculty of Science. A number of students completed their B. Sc., M. Sc. and Ph. D. theses.

AWARDS

Hrvoje Štefančić (on behalf of the Robin Hood development team consisting of Predrag Lazić, Hrvoje Abraham and Hrvoje Štefančić) was awarded “From Research to Enterprise” award by the Central European Initiative.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

1. Surfaces and nanostructures: Theoretical approaches and numerical calculations, Radovan Brako
2. Electronic properties of hybrid nanostructures, Željko Crljen
3. Electromagnetic field fluctuations: the van der Waals-Casimir forces, Marin-Slobodan Tomaš
4. Fundamental interactions in elementary particle physics and cosmology, Branko Guberina
5. Noncommutative spaces in high energy physics, Josip Trampetić
6. Matrix models, duality and field theory, Ivan Andrić
7. Quantum field theory, noncommutative spaces and symmetries, Stjepan Meljanac

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. Surfaces and nanostructures: Theoretical approaches and numerical calculations, Radovan Brako

Research, developmental and international projects

1. Fundamental questions of non-abelian quantum gauge theories and cosmology, Anđelka Andraši (collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Eötvös Loránd University, Budapest, Hungary)
2. Investigations on the Nature of Dark Matter and Dark Energy (DMDE), Neven Bilić (Scientific Joint Project 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. Hard-hadron physics in the standard model and beyond, Branko Guberina (collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and the Jozef Štefan Institute, Ljubljana, Slovenia)
4. QCD sum rules for exclusive decays of heavy hadrons, Blaženka Melić (International Research Project promoted by the Alexander von Humboldt Foundation)
5. Aspects of Calogero models, noncommutative geometry and quantum physics, Stjepan Meljanac (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. Nonabelian Cohomology and Applications in Geometry, Algebra and Physics, Zoran Škoda (collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Universität Hamburg, LMU München and Universität Göttingen, Germany)

SELECTED ORGANIZED CONFERENCES

1. 2nd Croatian-Hungarian Meeting – Fundamental Questions of Non-Abelian Quantum Gauge Theories and Cosmology, Rab, Croatia, August 30 – September 3, 2007, organized by I Dadić
2. Categories in Geometry and in Mathematical Physics, Split, Croatia, September 24-28, 2007, organized by I Baković and Z Škoda
3. Croatian-German Bilateral Symposium, DFG & NZZ (NSF) Workshop and Collaboration, Zagreb, Croatia, November 9-11, 2007, organized by J Trampetić.

SELECTED INVITED LECTURES

1. Baković I. Bigroupoid principal 2-bundles, Workshop on Higher categories and their applications, Toronto, Canada, January 9-13, 2007.
2. Trampetić J. Renormalizability of thera-expanded noncommutative gauge field theories, Conference on Noncommutative Spacetime Geometries, Alessandria, Italy, March 26-21, 2007.
3. Passek-Kumerički K. The 12th International Conference on Elastic and Diffractive Scattering: Forward Physics and QCD, Hamburg, DESY, Germany, May 21-25, 2007.
4. Nikolić H. Classical mechanics as nonlinear quantum mechanics, The conference Quantum Theory: Reconsideration of Foundations 4, Vaxjo, Sweden, June 11-16, 2007.
5. Bilić N. Thermodynamics of Dark Energy, III Southeastern European Workshop BW 2007 on Challenges Beyond the Standard Model, Kladovo, Serbia, September 2-9, 2007.
6. Škoda Z. Categorified actions and equivariance, International Symposium on Recent Advances in Mathematics and its Applications (ISRAMA 2007), Calcutta Mathematical Society, Kolkata, India, December 16-18, 2007.

SELECTED PUBLICATIONS

1. Bardek V, Feinberg J, Meljanac S. Collelctive field formulation of the multi-species Calogero model and its duality symmetries. Nuclear Phys B 2007: 767: 295.
2. Bardek V, Meljanac S. Waves and solitons in the two-family Calogero model. Phys Rev D 2007: 75: 127701.
3. Bilić N, Guberina B, Horvat R, Nikolić H, Štefančić H. On cosmological implications of gravitational trace anomaly. Phys Letters B 2007: 657: 232.
4. Das T K, Bilić N, Dasgupta S. Black-hole accretion disc as an analogue gravity model. JCAP 2007: 06: 0091.
5. Guberina B, Horvat R, Nikolić H. Nonsaturated Holographic dark energy. JCAP 2007: 0701: 012.
6. Crljen Ž, Baranović G. Unusual conductance of polyyne-based molecular wires. Phys Rev Lett 2007: 98: 116901.
7. Lazić P, Brako R, Gumhalter B. Structure and dynamics of Xe monolayers adsorbed on Cu(111) and Pt(111) surfaces studied in the density functional approach. Journal of Physics-Condensed Matter 2007: 19: 305004.
8. Nikolić H. Strings, T-duality breaking, and nonlocality without the shortest distance. Eur Phys J C 2007: 50: 431.
9. Kumerički K, Müller D, Passek-Kumerički K, Schäfer A. Deeply virtual Compton scattering beyond next-to-leading order: The flavor singlet case. Phys Letters B 2007: 648: 186.
10. Sambale A, Buhmann S Y, Welsch D-G, Tomaš M-S. Local-field correction to one- and two-atom van der Waals interactions. Phys Rev A 2007: 75: 042109.

Division of Experimental Physics

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

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 excellence in basic and applied research was maintained in the Division throughout 2007. A special effort was devoted to finding new sources of financing by exploiting the full integration into EU FP7 programs. The possibility to use other, diverse non-MZOS sources for financing for basic and applied physics has been thoroughly investigated. The effort has been successful, and a number of additional projects have been approved. After quite a number of years the major construction of new offices and laboratory space has started.

TOP ACHIEVEMENTS

Experimental high energy physics

The centrality and system size dependence of multiplicity fluctuations of charged particles in nuclear collisions at 158 A GeV was studied with the NA49 large acceptance detector at the CERN-SPS (Alt et al., 2007).

The energy dependence of electric charge correlations was studied with the Balance Function method in A+A collisions. In the mid-rapidity region, a decrease of the width of the Balance-Function distribution with increasing centrality of the collisions was observed (Alt et al., 2007).

The elliptic flow of Λ hyperons has been measured in semi-central Pb+Pb collisions. The observation of significant elliptic flow and its mass dependence suggest strong collective behavior of the matter produced in collisions of heavy nuclei already at the SPS (Alt et al., 2007).

The CMS potential for the observation and study of the $pp \rightarrow Z^0Z^0$ and $pp \rightarrow WZ^0$ reactions was investigated using fully simulated signal and background samples. Multiple gauge-boson production in pp collisions at LHC energies can be observed in the early phase of the experiment, with an integrated luminosity of 1 fb^{-1} or less was observed (Brigljević et al., 2007).

Nucleon-nucleon correlations

Multinucleon transfer reactions in $^{40}Ca+^{96}Zr$ and $^{90}Zr+^{208}Pb$ at energies close to the Coulomb barrier at the new large solid angle spectrometers coupled with gamma arrays were studied, such as the PRISMA+CLARA installed at Laboratori Nazionali di Legnaro, Italy. It has been shown that multinucleon transfer reaction mechanism strongly populates the states that belong to the particle(s)-phonon coupling scheme (Szilner et al., 2007).

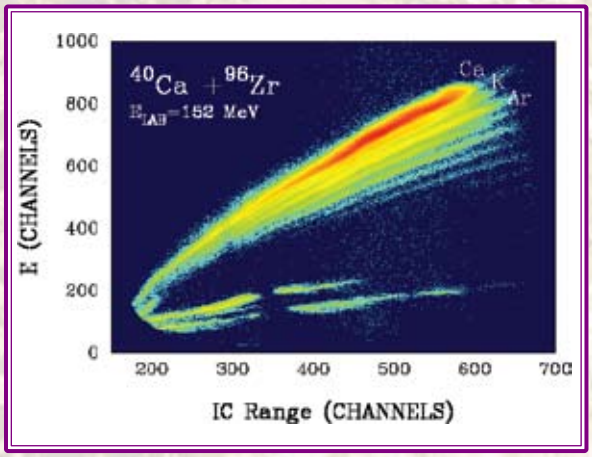

Figure 1: Example of two-dimensional Range - Total Energy matrix obtained in the reaction $^{40}Ca+^{96}Zr$. The most intense band corresponds to Z=20, i.e. isotopes of Ca.

Isospin and strange mesons near production threshold

As a possible probe of isospin effects in high-density nuclear matter the K^+ and K^0 strange meson production at 1.528A GeV was studied for the equal mass systems of $_{44}Ru+_{44}Ru$ and $_{40}Zr+_{40}Zr$, with the FOPI detector at GSI-Darmstadt. The measured double ratio $(K^+/K^0)_{Ru}/(K^+/K^0)_{Zr}$ was compared to the predictions of a thermal model and a relativistic mean-field transport model, using two different collision scenarios and under different assumptions of the stiffness of the symmetry energy. Good agreement was found with the thermal model prediction under the assumption of soft symmetry energy for infinite nuclear matter, while more realistic transport simulations of the collisions show a similar agreement with the data but also exhibit reduced sensitivity to the symmetry term (Lopez et al., 2007).

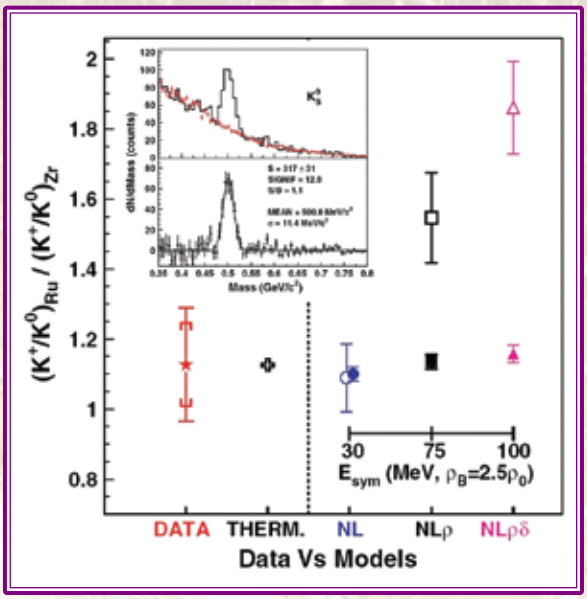

Figure 2: Experimental ratio $(K^+/K^0)_{Ru}/(K^+/K^0)_{Zr}$ (star) and theoretical predictions of the thermal model (cross) and the transport model with three different assumptions on the symmetry energy: NL (circles), NLρ (squares), and NLρδ (triangles), for two sets of calculations: open (full) symbols stands for infinite nuclear matter (heavy-ion collisions). Inset: Invariant mass spectra of π−π+ pairs.

Search for solar axions

The axion, a hypothetical elementary particle postulated by the Peccei-Quinn theory in 1977 to resolve the strong CP problem in quantum chromo dynamics, could

also explain the mystery of dark matter in the Universe. At CERN, scientists from our Laboratory for Electromagnetic and Weak Interactions are involved in the CAST experiment, designed to search for solar axions. CAST has recently reported an improved limit on the axion-to-photon coupling of 8.8×10^{-11} GeV^{-1}. For the first time, this is better than constraints from the energy balance in helium-burning stars (Andriamonje et al., 2007).

Figure 3: The CERN Axion Solar Telescope (CAST) experiment at CERN, which is looking for axions from the Sun.

OPERA neutrino oscillations experiment

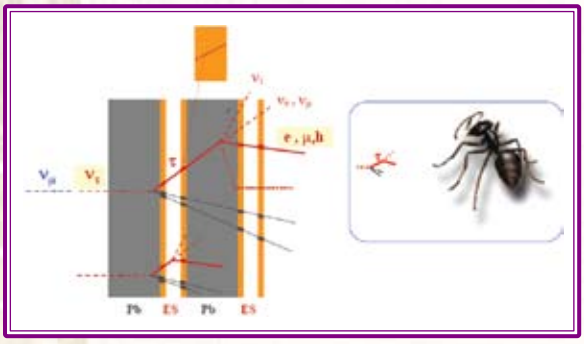

Figure 4: Topology of tau neutrino events in OPERA. These events would indicate oscillation between muon and tau neutrino flavours.

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 the veto system of the OPERA detector, which is placed at the underground Gran Sasso Laboratory, 732 km away from the CERN neutrino source. During 2007, our scientists have become members of the Slow control group and contributed in building the OPERA slow control system.

Dark energy models

Two most popular and viable dark energy models, based on vacuum decaying laws, appear to be largely compromised by transfer energy flux destabilization, suggesting that either a thermal equilibrium between vacuum and radiation never occurred, or that the dark energy models considered are in need of revision (Horvat and Pavon, 2007).

An observational hint of quantum gravity

Figure 5: The MAGIC gamma-ray telescope on La Palma in the Canary Islands.

The MAGIC gamma-ray telescope team studied two gamma-ray flares (observed on July 9, 2005) from the black hole at the heart of the galaxy Markarian 501 (over a half-billion-year away from Earth). They compared gammas in two energy ranges: from 1.2 to 10 TeV and from 0.25 to 0.6 TeV and found that higher-energy gamma rays arrived on Earth four minutes later than lower-energy ones. If the high-energy gammas really propagate

slower, it could be a way to constrain string theory or loop quantum gravity (Albert et al., 2007).

Natural isotopes in environmental studies and radiocarbon dating

Carbon exchange processes in atmosphere, water and lake sediments were studied and anthropogenic and/or natural influence to global and local level contamination has been determined by the measurement of ^{14}C and stable isotopes (^{13}C, ^{18}O, ^{14}N). Anthropogenic influence on water resources in Lika and Dalmatia has been assessed by using isotopic and chemical methods. Monitoring of ^{3}H activity in monthly precipitation in Croatia and Slovenia has been continued. A slight increase of ^{14}C activity in biological samples and atmospheric CO_2 in the immediate vicinity of the Nuclear Power Plant Krško during the exchange of fuel elements was observed. In the study of the two Starčevo culture sites near Slavonski Brod, the first absolute ^{14}C dates of the beginning of neolithization in Croatia were obtained (6070–4960 cal BC). The several periods of construction and repairs to the famous Mostar Bridge, spanning from the 12th to 18th century, were established (Obelic et al., 2007). Data on elastic scattering of electrons and positrons were critically reviewed in ICRU report 77 and will be used in dosimetry, radiotherapy and construction of spectrometers and radiation detectors.

NEW EQUIPMENT

Upgrade of ion microprobe

With the help of an IAEA funded project, a new quadrupole lens was added to the existing quadrupole doublet and a newly designed scattering chamber was installed. In such a way, the upgraded quadrupole triplet system provided a significantly better focusing capability of the facility (0.3 x 1 μm). By the installation of additional two quadrupole lenses planned for 2008 under the EU-FP6 project, our quintuplet system will be able to focus ions of up to 25 MeV (ME/Q2) rigidity.

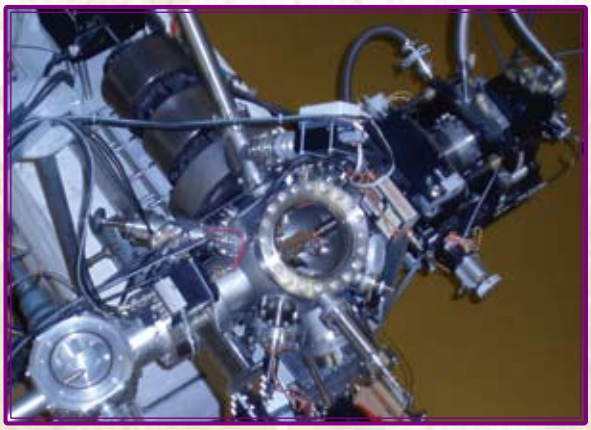

Figure 6: New scattering chamber installed at ion microprobe facility with quadrupole triplet configuration.

^{14}C dating by AMS

The new system for graphite preparation of micro-sized samples for ^{14}C measurement by AMS technique was constructed within the IAEA CRO/8/006 and EU FP6 AMS-^{14}C projects.

Figure 7: Vacuum line for preparation of graphite for ^{14}C AMS measurement technique.

Quantum Information Group

The Quantum Information Group has been formed in 2007. The activities include the building of a system for stochastic calculations and simulations utilizing the Quantum Random Number Generator (QRBG), built in 2005 by members of the group (http://random.irb.hr). A prototype of the Single Photon Detector was successfully tested at LMU Munich within the DAAD project "Experiments in quantum communication and quantum information". Our paper on QRBG, Rev. Sci. Instrum. 2007: 78: 045104:1-7, was chosen for reprint in Virtual Journal of Quantum Information.

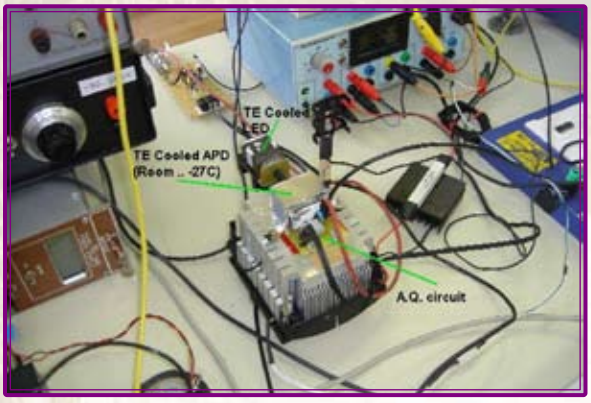

Figure 8: The Quantum Random Number Generator (QRNG).

Development of the tagged neutron inspection system for a cargo container inspection

A new tagged neutron system for the inspection of ship containers has been developed in the framework of the EURITRACK FP6 project. In the year 2007 the EURITRACK system has been installed and operated at the "Brajdica" container terminal of the Rijeka harbour. The neutron system is developed as an addition to the x-ray inspection system, which is a conventional method for ship containers. The neutron inspection system enables fast chemical analysis of suspicious volumes inside the container after being determined by x-ray scanning. The successfully performed tests at the Experimental Physics Neutron Laboratory of the Rudjer Boskovic Institute precede the field installation of the EURITRACK system. On the 31 May 2007, the EURITRACK system won the first price of Technological Innovation at the French Trophy of the Civil Defence of 2007 organized by High French Committee for the Civil Defence "to protect the future".

Figure 9: EURITRACK detection system at work implemented at the harbour Rijeka.

EDUCATION

In 2007 the members of the Division have been involved in lecturing undergraduate courses at the University of Zagreb (mostly at the Faculty of Science) and University of Rijeka, and graduate courses at the Faculty of Science of University of Zagreb, and at joint studies organized by RBI in cooperation with the Universities of Osijek and Dubrovnik.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

1. Experimental research of the nucleus: nuclear structures and reactions, Suzana Szilner
2. Ion beam interactions and nanostructures, Milko Jakšić
3. Hadronic physics and QCD, Ivan Supek
4. Heavy-ion physics, Zoran Basrak
5. Massive neutrinos and astro-particles: from particle physics to cosmology, Ante Ljubičić
6. Experimental physics at LHC energies, Krešo Kadija
7. Experiments in quantum communication and quantum information, Mario Stipčević
8. Photon-atom interactions and correlations, Tihomir Surić
9. Natural radioisotopes in investigation of karst ecosystem and dating, Bogomil Obelić
10. Prehistorical identity of first agricultural populations in continental Croatia, Kornelija Minichreiter
11. Development and application of nuclear analytical methods, Đuro Miljanić
12. Development of methods for control of illicit threat material trafficking, Dario Matika

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. High Energy Experimental Physics within and beyond the Standard Model, Krešo Kadija
2. Water in Karst - dynamics, geochemistry and isotopic processes, Bogomil Obelić

Research, developmental and international projects

1. Preparation of carbon samples for ^{14}C dating by the AMS technique – AMS-^{14}C, Ines Krajcar Bronić (EC FP6 program INCO-CT-2006-043584)
2. Upgrade of the RBI Tandem Accelerator Facility – RBI-AF, Stjepko Fazinić (EC FP6 program INCO Contract 043630)
3. EUROpean Nuclear Structure Integrated Infrastructure Initiative – EURONS, Zoran Basrak (EC FP6 program, Contract 506065)
4. TRAINMONHER - Valorization of Monumental Heritage through Higher Education and Professional Training. Socioeconomic study and analysis of National Policies on EU-MED-DEV countries and EC Directives, Bogomil Obelić (EC FP6 program INCO-CT-2006-518697)
5. EURITRACK, European illicit trafficking countermeasures kit, Vladivoj Valković (EC FP6 Specific Targeted Research or Innovation Project No. 511471)
6. Control of illicit trafficking in threat materials and humans, Vladivoj Valković (NATO project No. SfP 980526)
7. Nuclear techniques for the analysis and preservation of national heritage objects, Milko Jakšić (IAEA Technical Co-operation project, CRO/1/005)
8. Nuclear Techniques for the Protection of Cultural Heritage Artifacts in the Mediterranean Region, Stjepko Fazinić (National Coordinator, IAEA regional project RER/1/006)
9. Application of isotope techniques in investigation of water resources and water protection in the Karst area of Croatia, Nada Horvatinčić,. (IAEA Technical co-operation program CRO/8/006, co-operation with the University of Rijeka, Dept. of Physics, Faculty of Medicine)
10. Using Isotope Tracers as a Tool for Groundwater Vulnerability Assessment in the County of Split, Dalmatia, Nada Horvatinčić (IAEA Technical co-operation program CRO/8/007)
11. Isotope methods for management of drinking water resources, Nada Horvatinčić (IAEA regional project RER/8/012)
12. Measurements of differential cross sections for elastic scattering of ^{1}H and ^{4}He ions from selected light elements, Ivančica Bogdanović Radović (IAEA Research Contract 13269)
13. Heavy ion acceleration in 1.0 and 6.0 MV electrostatic accelerators, Milko Jakšić (IAEA Research Conract 13127)
14. Upgrade of PIXE and STIM imaging capabilities at Zagreb nuclear microprobe, Mladen Bogovac (IAEA Research Contract 13258)
15. Characterization of inorganic pigments used by selected painter(s) by nuclear microprobe, Stjepko Fazinić (IAEA Research Contract 13050)
16. Modification of electronic properties in insulators using nuclear microprobe, Marko

Karlušić (IAEA Research Contract 12925)
17. Improvements of ERDA technique using TOF spectrometer, Zdravko Siketić (IAEA Research Contract 14580)
18. Study of advantages and limitations of Si pin diodes as radiation detectors by ion beam methods, Milko Jakšić (bilateral project with Hungary)
19. Heavy ion physics, Roman Čaplar (International collaboration project RBI-KFKI Research Institute for Particle and Nuclear Physics, Budapest via Croatian (HAZU) and Hungarian Academy of Science)
20. Heavy-ion reaction dynamics studies, Zoran Basrak (bilateral research project Croatia-India)
21. OPERA collaboration, Ante Ljubičić (International collaboration between RBI, CERN, Geneva, Switzerland and LNGS , Gran Sasso, Italy)
22. Axion Solar Telescope (CAST) experiment, Milica Krčmar (International collaboration between RBI and CERN, Geneva, Switzerland on CERN)

SELECTED INVITED LECTURES

1. Antičić T. Search for a quark-gluon plasma, 5th Scientific Meeting of Croatian Physical Society, Primošten, Croatia, October 5 - 8, 2007.
2. Antičić T. Determining the best phenomenological model for hadron interactions using the anti-Omega to Omega ratio in proton-proton collisions, Astroparticle Physics: Current Issues (APCI07), Budapest, Hungary, July 21-23, 2007.
3. Basrak Z. Fusion of atomic nuclei, nuclear-session key talk at the 5th Scientific Meeting of Croatian Physical Society, Primošten, Croatia, October 5 - 8, 2007.
4. Bogdanović Radović I. Ion Beam Analysis - methodology and forensic applications, Joint IAEA ICTP Workshop: X-Ray Emission Techniques for Forensic Applications, Trieste, Italy, May 28 – June 1, 2007.
5. Fazinić S. Ion Beam Techniques for Analysis of Cultural Heritage Objects, VII International Conference on Science, Arts and Culture, Science for Cultural Heritage, Lošinj, Croatia, August 28-31, 2007.
6. Jakšić M. Remote accelerator experiments and education using accelerators, IAEA Technical Meeting: Enhancing nuclear science education and training using accelerators, Accra, Ghana, September 11-14, 2007.
7. Lakić B. Axions and Large Extra Dimensions, 3rd Joint ILIAS-CERN-DESY Axion-WIMPs training-workshop, Patras, Greece, June 19-25, 2007.
8. Milin M. Clustering in light nuclei studied with ^{6}He beam, CLUSTERS' 2007, Stratford upon Avon, England, September 3-7, 2007.
9. Sudac D. Discrimination of the explosives from other materials by using the tagged neutron beam, NATO Advanced Research Workshop on ''Detection of Liquid Explosives and Flammable Agents in Connection with Terrorist Actions'', Saint-Petersburg, Russia, October 17-19, 2007.
10. Švarc A. On Ambiguities and Uncertainties in PWA, 11th International Conference on Meson-Nucleon Physics and the Structure of the Nucleon (MENU2007), September 10-14, 2007, IKP, Forschungzentrum Juelich, Germany.

SELECTED PUBLICATIONS

1. Summers NC, Pain SD, Orr NA, Catford WN, Angelique JC, Ashwood NI, Bouchat V, Clarke NM, Curtis N, Freer M, Fulton BR, Hanappe F, Labiche M, Lecouey JL, Lemmon RC, Mahboub D, Ninane A, Normand G, Nunes FN, Soić N, Stuttge L, Timis CN, Thompson IJ, Winfield JS, Ziman V. B(E1) strengths from Coulomb excitation of ^{11}Be. Phys Lett B 2007: 650:124.
2. Horvat R, Pavon D. Constraining interacting dark energy models with flux destabilization, Phys. Lett. B 2007: 653: 373
3. Alt C et al. (NA49 Collaboration-IRB: Antičić T, Kadija K, Nikolić V, Šuša T): Elliptic flow of Lambda hyperons in Pb+Pb collisions at 158AGeV. Phys Rev C 2007: 75: 044901.
4. Szilner S,.. Soić N. et al. (PRISMA+CLARA-RBI collaboration): Multinucleon transfer reactions in closed-shell nuclei. Phys Rev C 2007: 76: 024604.
5. Lopez X, et al. (FOPI Collaboration-IRB: Basrak Z, Čaplar R, Gašparić I, Kiš M Korolija M). Isospin dependence of relative yields of K^+ and K^0 mesons at 1.528A GeV. Phys Rev C 2007: 75: 011901(R).

6. Andriamonje S et al. (RBI-CAST collaboration: K. Jakovčić, M. Krčmar, B. Lakić, A. Ljubičić): An improved limit on the axion-photon coupling from the CAST experiment, JCAP 2007: 04: 010.
7. Brigljević V, Ferenček D, Morović, S et al. Study of di-boson production with the CMS detector at LHC. J Physics G 2007: 34: 269.
8. Kaliman Z, Pisk K, Surić T. Perturbative calculation of the cross section in double ionization by high-energy Compton scattering , European Phys JD: 2007:42: 369.
9. Sudac D, et al. Identification of materials hidden inside a sea-going cargo container filled with an organic cargo by using the tagged neutron inspection system. Nucl Instr Meth B 2007: 261: 321.
10. Jakšić M, Medunić Z, Skukan N, Bogovac M, Wegrzynek D. Fabrication of a Si photodiode for position sensitive radiation detection. IEEE Trans Nucl Sci 2007: 54:280.
11. Obelić B, Krajcar Bronić I, Barešić J, Peković Ž, Milošević A. Dating of the Old Bridge in Mostar, Bosnia and Herzegovina. Radiocarbon 2007: 49: 617.
12. Albert J, Hrupec D, et al. Variable very high energy gamma-ray emission from Markarian 501, Astrophys. J: 2007: 669: 862.

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 Division of Materials Physics is focused on fundamental and applied studies of physical parameters and processes that describe and connect the microscopic, mesoscopic and macroscopic properties of condensed matter and molecules. Nanoscience and nanotechnology has been the most active direction of both fundamental scientific research and developments in technology. Various kinds of nanophased materials have been produced by non-equilibrium thermodynamic processing (magnetron sputtering, ion implantation) and subsequent treatments. The structure of these materials has been examined by different methods, including XRD, SAXS, Raman spectroscopy, electron microscopy, AFM etc., and the measured physical properties were correlated with the respective findings. Fundamental research in the field of molecular and solid state physics placed 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 strongly nonlinear effects in laser-matter interaction, and the spontaneous and induced self-organization in condensed systems continue to be subjects of intensive research. During 2007, the results of investigations carried out in the Division were published in 35 contributions to journals listed in current contents, with an average impact factor per paper of 1.91.

TOP ACHIEVEMENTS

Dislocation-related deep levels in carbon rich p-type polycrystalline silicon

Dislocation-related defects in p-type silicon crystals grown by the edge-defined film-fed growth (EFG) and float-zone method were studied by the deep level transient spectroscopy (DLTS) technique. The complex behaviour of defects in EFG material suggests that

dislocations are either decorated with clouds of carbon-related or metallic defects, or the close spacing produces overlap of space-charge regions, therefore affecting the electrical activity (Capan et al., 2007).

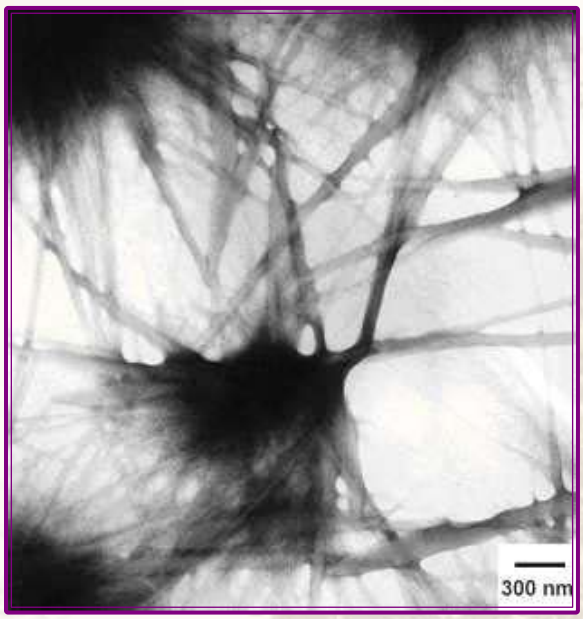

Figure 1: DLTS spectra of dislocated float-zone (FZ) and carbon-rich polycrystalline edge-defined film-fed grown (EFG) silicon samples.

Amorphous-nanocrystalline silicon thin films

The nano-structure of thin Si films was examined by Raman spectroscopy and GISAXS analysis as a function of deposition conditions in the RF PECVD reactor. The GISAXS scattering patterns indicate the presence of 'particles' in the 'bulk' of thin films, with gyration radii in the range of 2 to 5 nm that could be attributed to nano-crystals embedded in amorphous matrix (Figure 2). Samples which had been deposited with higher discharge power and lower silane fraction had larger particles and increased surface roughness (Gracin et al., 2007).

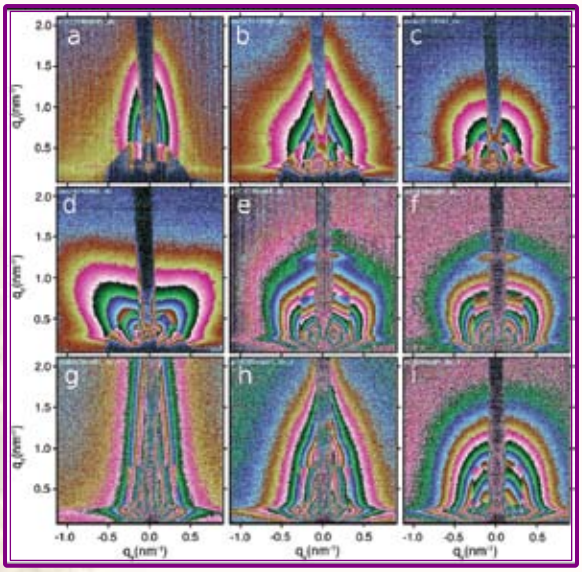

Figure 2: 2D GISAXS patterns obtained from nanocrystalline-amorphous Si thin films deposited on different substrates (a,d,g), and from samples deposited under conditions that favours "transport limited growth" (b,e, f, h) or "strong plasma surface interactions" (c, i)).

Thermal expansion of Cr-doped mullites derived from single-phase precursors

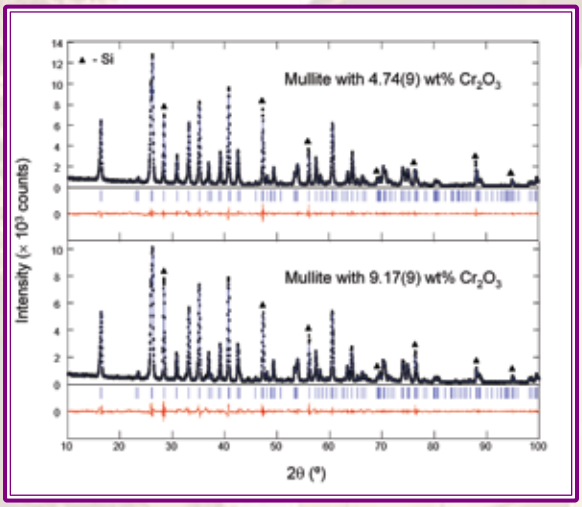

Figure 3: Results of the WPPF procedure in precise determination of unit-cell parameters for selected Cr-doped mullites, with Si powder as internal standard at RT.

Nanocrystalline powders of mullite containing 0, 2.30, 4.74, 6.97 and 9.17 wt% of Cr_2O_3 were derived from single-phase precursors, and their thermal expansion between 480 and 940 ºC was studied by in-situ XRD. Unit-cell parameters were precisely determined using the whole-powder-pattern fitting (WPPF) method. Both undoped and Cr-doped mullites displayed the strongest thermal expansion along the b-axis, followed by c and then a. Coefficients of thermal expansion along the a, b and c axes displayed minima for mullite doped with 6.97 wt% Cr_2O_3 (Gržeta et al., 2007).

Catalytic activity of nanocrystalline nickel thin films

The grain-size of Ni-particles in sputter-deposited thin films (400 nm) was controlled by the substrate temperature. It was found that nc-Ni catalytic activity for the hydrogen evolution reaction correlates well with the ratio between the nanocrystalline (d) and non-homogeneus disordered (R_G) fraction of the nc-Ni film as determined by the XRD and GISAXS analyses. The catalytic activity of nanocrystalline nickel was markedly greater at larger fraction of the isotropic inhomogenities inside the film (Metikoš-Huković et al., 2007; Radić et al., 2007).

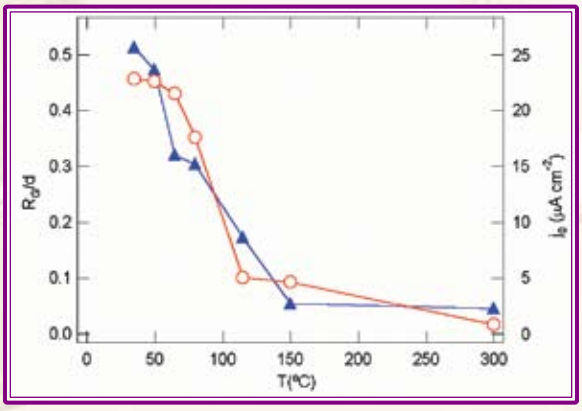

Figure 4: The exchange current density (j_0) for hydrogen evolution reaction and ratio R_G/d versus substrate temperature, T_S, dependence for sputter deposited nc-Ni films.

A new method for the determination of the phase-transition pressure in crystals

A new method for determination of the phase-transition pressure in crystals, with a small volume change, was presented. Lattice dynamics calculations, within the framework of perturbation density functional theory (PDFT) were performed. By monitoring the phonon frequencies as a function of pressure it is possible to determine the pressure of the phase transition. It is the pressure at which a particular phonon frequency goes to zero, i.e., the lattice become unstable. The method was applied to locate the phase-transition pressure in the crystals of ZnS, ZnSe, CdS, and CdSe. The calculated transition pressures were in much better agreement with experiments than previous calculations (Kirin et al., 2007).

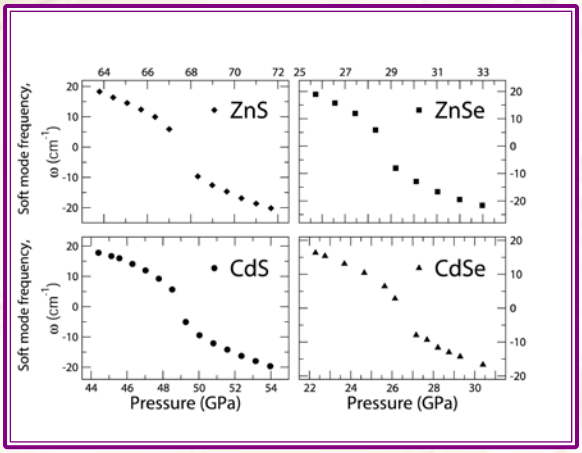

Figure 5: Pressure dependence of the soft-mode frequency for selected materials.

New features of acetylacetone captured by solid-state Raman spectroscopy

Low temperature Raman spectra of acetylacetone, an organic molecule with an intramolecular hydrogen bond, revealed unusually strong broad bands whose intensities change with temperature and the

wavelength of the exciting line. These broad bands corresponded to transitions from a mixed triplet-singlet electronic state lying approximately 20000 cm^{-1} (2.5 eV) above the ground state. In the free molecule, there was only a pure triplet state at this energy, and it could not be reached by photon excitation. In solid acetylacetone, this state, whose lifetime is extended by freezing, had a mixed singlet/triplet character. These characteristics enabled the observation of transitions to various conformers in the ground state (Mohaček Grošev et al., 2007).

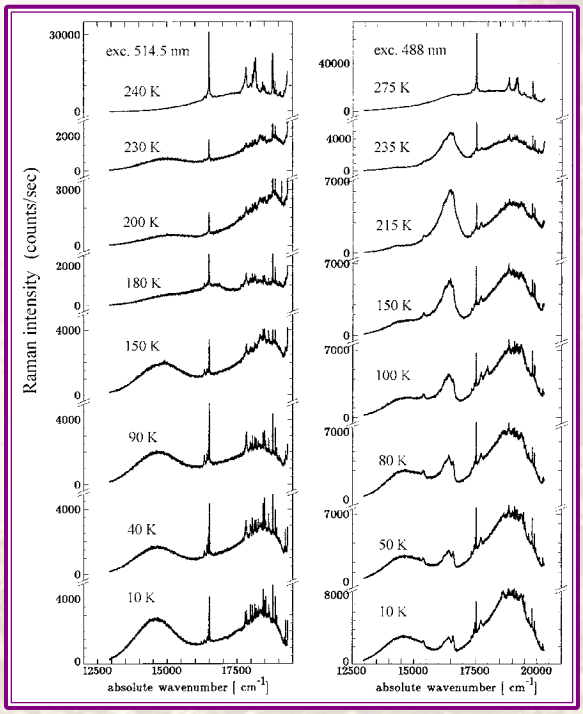

Figure 6: Low temperature Raman spectra of acetylacetone reveal unusually strong broad bands, which correspond to transitions from an excited mixed triplet-singlet electronic state into the ground states of various conformers.

Flow instability of fluid-metal layer generated by laser pulse on an inclined metal surface

It was found that nanosecond laser–matter interaction with metal surfaces under an angle causes the formation of nonlinear micron-scale waves and localized structures resembling the gravitationally caused flow structures on an inclined plate. Juxtaposition of experimentally generated structures with those simulated numerically, on the basis of the equation derived by A.L.Frenkel, showed a very good qualitative agreement. The experiments confirmed the dependence of the structure evolution on the laser power profile and on the irradiation angle. These results were judged by the referees to constitute ”an important paper” (Lugomer et al., 2007).

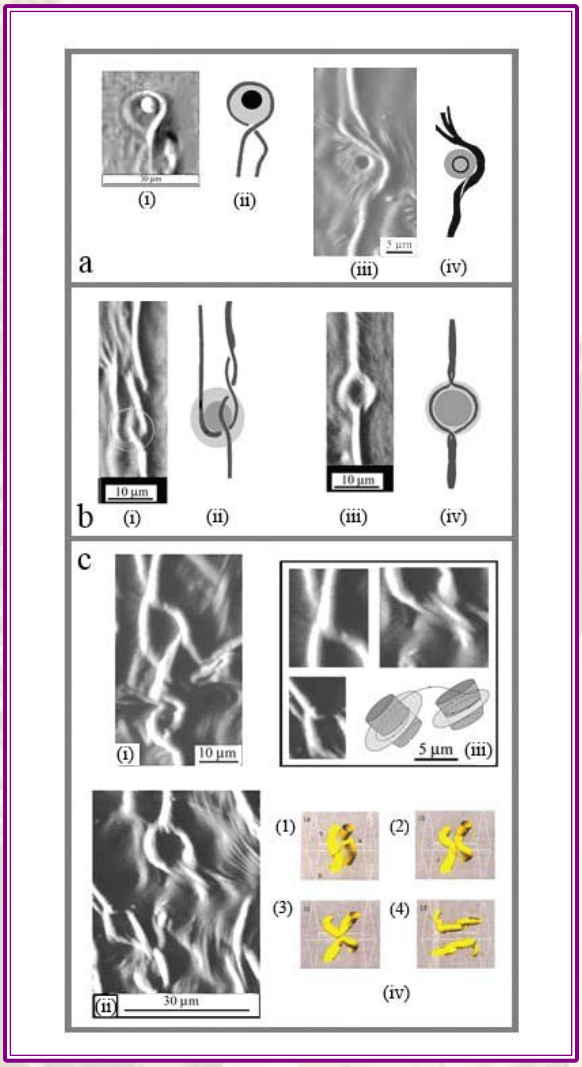

Figure 7: Comparative view of the optical micrographs of surface flow structures in various regions of the spot on very pure Ti, irradiated under θ=20° and of numerical simulation based on the Frenkel model.

Polymer electrolyte for Zn rechargeable nanostructured galvanic cells.

The effects of adding nanosized TiO_2 grains to $(PEO)_8ZnCl_2$ polymer electrolytes, as well as the influence of γ-radiation, were studied by small-angle X-ray scattering (SAXS), simultaneously recorded with differential scanning calorimetry (DSC). These treatments largely enhanced the conductivity of the polymer electrolyte. A room-temperature conductivity increase of up to two orders of magnitude was achieved. Addition of nanograins increased conductivity more than can be ascribed to crystallinity, possibly because of interactions of the anion with nanograins (Turković et al., 2007).

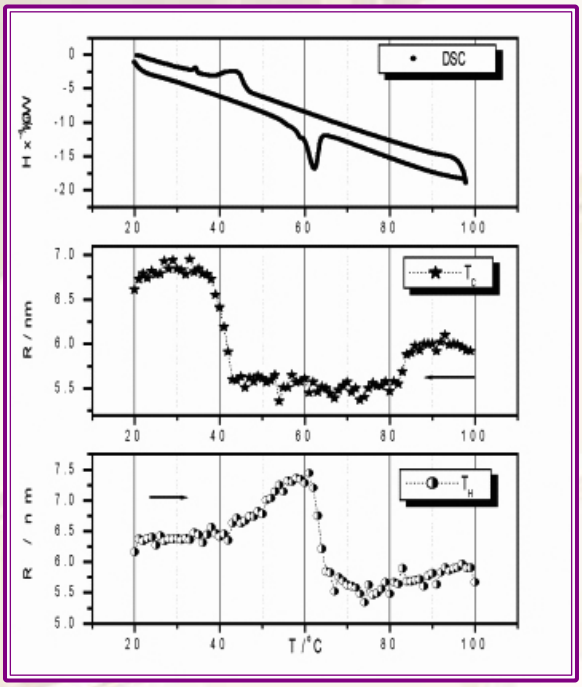

Figure 8: DSC (top panel) and SAXS (lower panels - heating and cooling cycles) of $(PEO)_8ZnCl_2$ irradiated with γ-rays of 309 Kgy.

EDUCATION

Members of the Department of Materials Physics teach 7 graduate and 7 postgraduate courses of physics and related topics at the Faculty of Sciences, Faculty of Electrical Engineering and Computing, Faculty of Chemical Engineering and Technology in Zagreb and elsewhere.

AWARDS

Ivana Capan, senior assistant with the Division of Materials Physics, received the Annual National Award for young scientist for 2007 for her research in the field of defects in semiconductors - the most prestigious scientific recognition for young scientist available in Croatia.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

1. Synergy of nanophases and nanocomposites, Aleksandra Turković
2. Basic properties of nanostructures and defects in semiconductors and dielectrics, Branko Pivac
3. Doped optoelectronic and ceramic nanomaterials, Biserka Gržeta
4. The thin film silicon alloys on the amorphous to crystalline transition, Davor Gracin
5. Thin Films of Novel Amorphous or Nanostructured Materials, Nikola Radić
6. Semiconductor materials for optoelectronics and nonotechnology, Branko Šantić
7. Physics and application of nanostructures and bulk matter, Krešimir Furić
8. Organizational processes and optical interactions in condensed molecular systems, Stjepan Lugomer

Program supported by the Ministry of Science, Education and Sports

1. Advanced materials and applications for energy conversion and storage, Branko Pivac

Research, developmental and international projects

1. Study of nanocomposite polymer electrolytes, Aleksandra Turković, (Croatia-Slovenia).
2. Study of disordered materials, nano-optical layers, Mile Ivanda, (Croatia-Slovenia).
3. Research of defects in Si and Ge induced by fast neutrons, Branko Pivac (Croatia-Slovenia).
4. Quantum effects in vibrational states of nanocrystalline silicon, Davor Gracin (Croatia-Slovenia).
5. Thin ZnO layer optimization in amorphous silicon PV cells, Davor Gracin, (Croatia-Macedonia).
6. Laser-induced surface self-organization: formation of surfaces with special properties, Stjepan Lugomer (Croatia-Hungary).
7. Ion beam modifications of SiC for elelctronic and optoelectronic applications, Branko Šantić (Croatia-Hungary).
8 Research on silicon and germanium nanostructures, Branko Pivac, (COGITO - Bilateral collaboration with France).
9. LPMAS, Davor Gracin (EU- FW6 -INCO-Project No FP6-509178).
10. RISE, Uroš V. Desnica (EU-FW6-INCO-Project No FP6-509161).
11. Hybrid photovoltaic module, Davor Gracin (Ministry of Science, Education and Sport-HITRA-STIRP Project TP-02/0098-35).
12. The origin of structural defects and their effects upon the properties if silicate glass, Davor Gracin, (National Science Foundation of Croatia).

SELECTED INVITED LECTURES

1. Armellini C, Biljanović P, Chiappini A, Chiasera A, Ferrari M, Ivanda M (lecturer); Jestin Y, Mattarelli M, Minati L, Montagna M, Moser E, Nunzi Conti G, Pelli S, Righini CG, Speranza G, Tosello C. Nanocomposite Photonic Glasses and Confined Structures Tailoring Er^{3+} Spectroscopic Properties, MIPRO 2007 30^{th} International Convention, Opatija, Croatia, May 25, 2007.
2. Turković A. SAXS Characterization of Mesoporous Thin Films: A Brief Review. E-MRS 2007 Fall meeting, Warszaw, Poland, September 17-21, 2007.

SELECTED PUBLICATIONS

1. Lugomer S, Maksimović A, Peto G, Karacs A. Flow instability of fluid-metal layer generated by laser pulse on an inclined metal surface: Experiments and simulation. Appl Phys Lett 2007: 90: 091917
2. Metikoš-Huković M, Grubač Z, Radić N, Dubček P, Djerdj I. The influence of local structure of nanocrystalline Ni films on the catalytic activity. Electrochem Comm 2007: 9: 299
3. Kirin D, Lukačević I. Stability of high-pressure phases in II-VI semiconductors by a density functional lattice dynamics approach. Phys Rev B 2007: 75: 172103
4. Mohaček-Grošev V, Furić K, Ivanković H. Luminescence and Raman spectra of acetylacetone at low temperatures. J Phys Chem A. 2007: 111: 5820
5. Gašparović B, Risović D, Ćosović B, Nelson A. The Influence of Frequency on Fractal Dimension of Adsorbed Layers. Electrochim Acta 2007: 52: 2527
6. Radić N, Dubček P, Bernstorff S, Djerdj I, Tonejc AM. Structural study of nanocrystalline nickel thin films. J Appl Cryst 2007: 40: 377
7. Gracin D, Bernstorff S, Dubček P, Gajović A, Juraić K. Study of mixture amorphous-nanocrstalline thin silicon films by GISAX spectroscopy. J Appl Crys 2007: 40: 373
8. Lugomer S, Fukumoto Y, Farkas B, Szorenyi T, Toth A. Super-complex wave-vortex multiscale phenomena induced in laser-matter interactions. Phys Rev E. 2007: 76: 1
9. Turković A, Pavlović M, Dubček P, Lučić-Lavčević M, Etlinger B, Bernstorff S. SAXS/DSC study of polymer electrolyte for Zn rechargeable nanostructured galvanic cells. J Electrochem Soc 2007: 154: 554
10. Capan I, Borjanović V, Pivac B. Dislocation-related deep levels in carbon rich p-type polycrystalline silicon. Sol Energy Mater Sol Cells 2007: 91: 931
11. Lučić Lavčević M, Dubček P, Turković A, Crnjak-Orel Z, Bernstorff S. Nanostructural depth-profile of vanadium/cerium oxide film as a host for lithium ions. Sol Energy Mater Sol Cells 2007: 91: 616
12. Turković A, Orel B, Lučić-Lavčević M, Dubček P, Crnjak-Orel Z, Bernstorff S. GISAXS study of temperature evolution in nanostructured $CeVO_4$ films. Sol Energy Mater Sol Cells 2007: 91: 1299

Division of Laser and Atomic Research and Development

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

DIVISIONAL ORGANIZATION

Head: 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

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, photonics and the fundamentals of optical thin films. Besides this, 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: development of photodynamic devices; development of multicomponent optical systems and development of new MediLED device for photodynamic therapy. These devices and systems will have use in the medical field, particularly new instrumentation for photodynamic diagnosis and therapy of malignant skin diseases.

TOP ACHIEVEMENTS

Optical thin films

The research tasks in the field of optical coatings were initially addressed towards the modelling of thin film mixtures using effective medium theories. These theories are often

successfully used to account for the refractive index of a mixture. However, the analysis of spectrophotometric data of niobia-silica mixtures has shown that such theories fail to describe the variation of the absorption coefficient with the material composition. In this context, we have studied various films with an in-depth variation of the composition. Based on the results, a characterization of complex coatings consisting of combinations of films of linearly varying and constant composition, i.e. rugate filters, has been performed using spectrophotometric and ellipsometric data. The results demonstrated the high sensitivity of ellipsometry for characterization of the refractive index profile. In addition, during the last months of 2007, metal island films have been produced and studied. Due to the surface plasmon resonance, the peculiar optical performance of these films incorporated into dielectric multilayer structures may enable novel designs of optical coatings in future.

Blind signal processing

Research activities in the area of signal processing were focused on areas such as: model-free single-sensor blind signal deconvolution; sparse component analysis with application in underdetermined blind source separation; and compressive sampling with

application in unsupervised segmentation of low-dimensional multispectral images.

Photodynamic diagnosis and therapy

In 2007, the development and testing of an advanced apparatus for photodynamic diagnosis and therapy (PDT and PDD) of malignant skin diseases under the brand name - MediLED-7® continued. The device was completed with new software. The development of a new device MediLED-8® has started.

PATENTS

A patent application, entitled "Intelligent sequential illuminating device for photodynamic therapy", was filed on 19 April 2007. The application received a positive written opinion as well as the publication number WO/2007/119084.

NEW EQUIPMENT

1. Digital Lock-in amplifier Signal Recovery - EG&G 7265.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Analysis of multispectral data, Ivica Kopriva

EDUCATIONAL ACTIVITIES

Members of the Division teach courses on Faculty of Electrical Engineering, University of Osijek, and in Polytehnic Velika Gorica, Velika Gorica, Croatia.

SELECTED INVITED LECTURES

1. Kopriva I. Blind separation of statistically dependent sources, Technical University Berlin, Faculty of Electrical Engineering and Computer Science, Institute of Energy and Automation Technology, Electronic and Medical Signal Processing Group, Berlin, Germany, October 11, 2007.
2. Kopriva I. Blind separation of statistically dependent sources, The George Washington University, School of Engineering and Applied Science, Department of Electrical and Computer Engineering, Washington D.C., USA, September 21, 2007.

SELECTED PUBLICATIONS

1. Janicki V, Sancho-Parramon J, Stenzel O, Lappschies M, Görtz B, Rickers C, Polenzky C, Richter U. Optical characterization of hybrid antireflective coatings using spectrophotometric and ellipsometric measurements. App Optics 2007:46: 6084.
2. Kopriva I, Seršić D. Wavelet packets approach to blind separation of statistically dependent sources, Neurocomputing 2007:10:106.
3. Wasylkiwskyj W, Kopriva I, Doroslovački M. Image frequency suppression in frequency-scanned direction-of-arrival estimation systems. IET Proc Radar Sonar Navigation 2007:1:191.
4. Kopriva I. Approach to blind image deconvolution by multiscale subband decomposition and independent component analysis, JOSA A 2007:24:973.
5. Wasylkiwskyj W, Kopriva I, Doroslovački M, Zaghluol A. A new root–based direction finding algorithm. Radio Sci 2007: 42: RS2S90.
6. Kopriva I, Peršin A, Zorc H, Lipozenčić J, Pašić A, Kostović K, Lončarić M. Visualization of basal cell carcinoma by fluorescence diagnosis and independent component analysis, Photodiagnosis Photodyn Ther 2007:4:190.
7. Turković A, Pavlović M, Dubček P, Lučić-Lavčević M, Etlinger B, Bernstorff S. SAXS/DSC study of polymer electrolyte for Zn rechargeable nanostructured galvanic cells. J Electrochem Soc 2007:154: A554.

Chapter in Book

1. Zorc H. Croatia and European Research Area, Contemporary Croatian Topics, Croatian System Society (in Croatian) Zagreb 2007, ISSN-1846-6451.

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

OVERVIEW OF THE DIVISION

The Division of electronics continues to work on the research and development of novel intelligent data and signal analysis techniques and their application in biomedicine, computational biology and bioinformatics, as well as on the development of advanced measurement techniques. The strong multi-disciplinary orientation was confirmed this year with an impressive publication record in different fields.

In 2007, the Division was granted a long-term research program entitled “Computational knowledge discovery in scientific applications (PI Dragan Gamberger), financed by the Croatian Ministry of Science, Education and Sports. The research program involves 5 related research projects, three of them from within the Division, including a number of researchers from different academic institutions of the University of Zagreb.

Besides these scientific projects, the Division works on a number of international multilateral (FP6 project HEARTFAID) and bilateral projects. The laboratory for stochastic signals and processes started collaboration with the Končar Institute for Electrical Engineering on the reliability of programmable logic devices in industrial embedded systems.

Our researchers contribute to higher education by providing both undergraduate and postgraduate courses at the University of Zagreb.

TOP ACHIEVEMENTS

Knowledge discovery methodology and applications

A new technique, called iterative subgroup discovery, has been developed and applied for data analysis of patients suffering from brain ischemia (Gamberger et al., 2007). Advanced data mining methodology has also been applied for intelligent analysis of the data collected under the clinical study of posttraumatic stress disorder.

A complex knowledge discovery procedure, including a sequence of data processing and filtering algorithms together with support vector regression model development, has been designed and successfully applied to the estimation of anti-tumour activity in tumour cell lines (IC50 values, in-vitro testing) for a series of crown ether compounds.

Meta-modelling of complex real-world processes using machine learning algorithms and data mining tools is a relatively unexplored field. An application to the problem of so called dose-rate buildup factors in radiation protection has proved the potential and advantages of the machine learning paradigm in formulating accurate and reliable approximate models of complex processes (Trontl et al., 2007).

Knowledge representation and reasoning for healthcare

Figure 1. WEB-prototype of the OWL based reasoner – CWI, a plug-in component for the Protege ontology editor, operating on heart failure ontology and patient records captured from local clinic patient records.

Within the activities related to the HEARTFAID project (EUFP6 ICT-STREP) focused on the research and development of a knowledge-enabled platform for the support of healthcare for elderly patients suffering from heart failure syndrome. The laboratory for information systems is leading work package 4 – Knowledge representation, discovery and management. During the second year, our focus was on the definition of knowledge representation and formulation of ontology for the heart failure domain. Within this activity, a new ontology reasoner-interpreter called CWI, based on the OWL language (Ontology Web Language) has been built for testing the new heart failure disease ontology, and as a prototype for the decision support services of the HEARTFAID platform (see Fig. 1).

Advanced measurement systems and signal processing techniques

A numerical procedure for the computation of natural gas molar heat capacity, the isentropic exponent, and the Joule-Thomson coefficient has been derived using fundamental thermodynamic equations, DIPPR AIChE generic ideal heat capacity equations, and AGA-8 extended virial-type equation of state. The procedure enables precise calculation of natural gas properties and can be efficiently applied to flow-rate measurements (Marić I, 2007). Focus was also given to the development of new methods for fractal-feature extraction from time series based on data embedding in pseudo phase space, where trajectory vector projection on principal axes reveals scale-invariant statistics. The method is illustrated on a human heartbeat time series (interbeat interval). An ongoing research activity in the signal processing field is the development of an integrated approach for the quantification of recurrences in short sequences. Coupling of the so called Recurrence Quantification Analysis technique, with machine learning algorithms, into a new soft-

ware system will enable automated analysis of short sequences or signals (from few tens to a few hundred points), involving simultaneous optimization of the RQA transform with respect to the particular annotation/classification problem (such as protein sequences, heart rate variability analysis, etc.).

EDUCATION

In 2007 the memebers of the Division lectured one course at the PhD Program of the Medical School (University of Zagreb) and the other one at the PhD Program of the Faculty of Electrical Engineering and Computing (University of Zagreb). They also lectured two courses at the Graduate Program of the Faculty of Electrical Engineering and Computing (University of Zagreb).

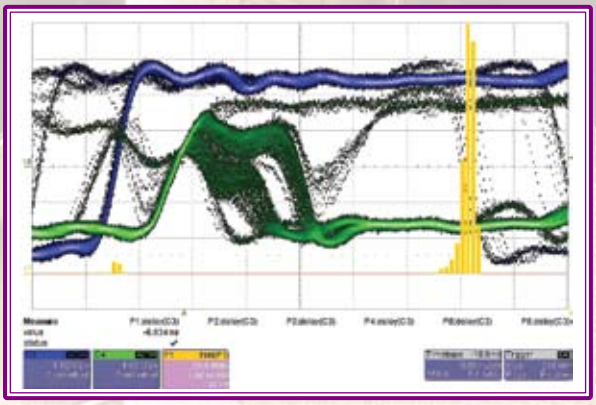

Figure 2. Time response (or propagation delay) of a metastable flip-flop. Results were obtained within the scope of the R&D collaboration with the Končar Institute for Electrical Engineering.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

1. Machine Learning Algorithms and their Application, Dragan Gamberger
2. Computational Intelligence Methods in Measurement Systems, Ivan Marić
3. Real Life Data Measurement and Characterization, Branka Medved Rogina

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. Computational knowledge discovery in scientific applications, Dragan Gamberger

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. Intelligent Data Analysis, Dragan Gamberger (Croatian-Slovenian bilateral project)
3. Inductive Databases for Genomics and Proteomics, Tomislav Šmuc (Croatian-Slovenian bilateral project)
4. Reliability of programmable logic devices in industrial embedded systems, Branka Medved Rogina (R&D project with the Končar Institute for Electrical Engineering)

SELECTED PUBLICATIONS

1. Gamberger D, Lavrač N, Krstačić A, Krstačić G. Clinical data analysis based on iterative subgroup discovery: Experiments in brain ischaemia data analysis. Appl Intell 2007: 27: 205.
2. Trontl K, Šmuc T, Pevec D. Support vector regression model for the estimation of γ -ray buildup factors for multi-layer shields. Ann Nucl En 2007: 34: 939.
3. Stipčević M, Medved Rogina B. Quantum random number generator based on photonic emission in semiconductors. Rev Sci Instrum 2007: 78: 45104.
4. Marić I. A procedure for the calculation of the natural gas molar heat capacity, the isentropic exponent, and the Joule-Thomson coefficient. Flow Meas Instrum 2007: 18: 18.
5. Marjanović M, Kralj M, Supek F, Frkanec L, Piantanida I, Šmuc T, Tušek-Božić Lj. Antitumor Potential of Crown Ethers: Structure-Activitiy Relationships, Cell Cycle Disturbances, and Cell Death Studies of a Series of Ionophores. J Med Chem 2007: 50: 1007.

Division of Physical Chemistry

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

DIVISIONAL ORGANIZATION

Head: Aleksandar Sabljić

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

OVERVIEW OF THE DIVISION

In 2007, members of the Division published nearly 50 contributions in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical chemistry, the modelling of physical and chemical processes, structural and chemical analyses, and in biosciences. A significant part was published in the highest ranking journals such as: Journal of Medicinal Chemistry, Current Medicinal Chemistry, Advanced Materials, Proteins, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of the American Society for Mass Spectrometry, and Physical Review B. A large fraction of those contributions were carried out within domestic (50%) and international (45%) collaborations. The high proportion of fruitful international collaborations demonstrates the strong presence of the Division in the European Research Area. Division members also contribute extensively (30 courses) to undergraduate and graduate education in Croatia. Finally, as is the case every year, the division members have organized several well-attended international conferences and workshops, such as the traditional 22nd MATH/CHEM/COMP and the 2nd Opatija Meeting on Computational Solutions in the Life Sciences.

TOP ACHIVEMENTS

Double proton transfer in the formic acid dimer

The formic acid dimer (FAD) is a prototype for studying double hydrogen bonded systems. The time constant of its proton transfer has been measured in 2002 for the first time. However, there was a controversy concerning the assignment of tunnelling splittings in the vibrational ground state and the asymmetric CO-stretching excited state, i.e. does the excitation of the CO-vibration promote or

hinder tunnelling. We have addressed this issue by solving the five-dimensional reaction space Hamiltonian and have obtained a tunnelling splitting 2.4 times larger in the ground state than in the CO-stretching excited state (Matanović et al., 2007). Thus, it was demonstrated that vibrational excitation does not always promote tunneling. The most recent experiments supported our conclusion.

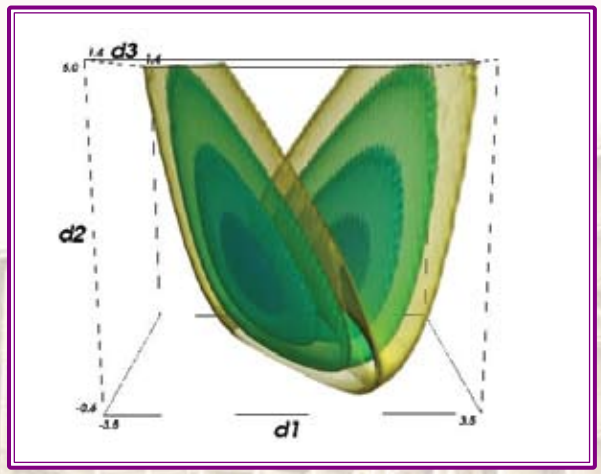

Figure 1. 3D crossection of the five dimensional potential energy surface of the formic acid dimer. The isosurfaces correspond to energies at 800, 2000, 4000 and 6000 cm^{-1}.

Interactions of Ras proteins with their effectors

Knowledge about interactions between Ras proteins (Ras, Rap…) and their effectors is important from both the biological and medicinal points of view. Ras belongs to the superfamily of small GTP binding proteins. Due to its ability to fluctuate between active (GTP bound) and inactive (GDP bound) states, it acts as a switch in many cellular pathways. Certain mutations block this function leading to a disease. We have found that the interactions between Ras and its effectors Raf and RalGDS are electrostatically driven (Tomić et al., 2007). 3D QSAR models were derived for predicting binding affinities of mutant proteins and the potential binding sites were determined for small molecules that can either prevent binding of an effector or help to increase selectivity of Ras toward a particular effector.

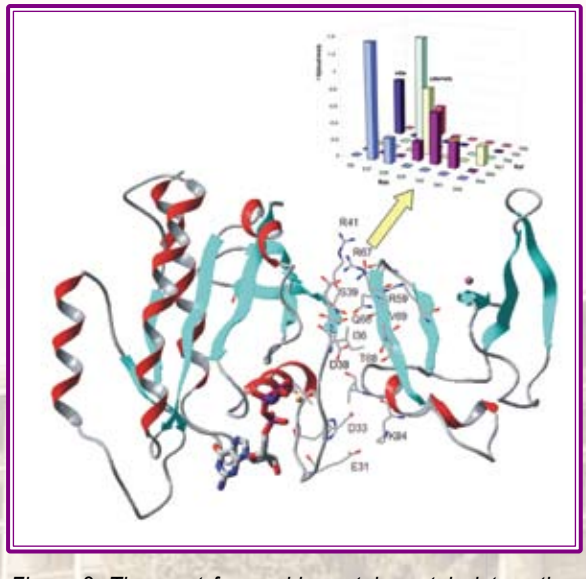

Figure 2. The most favourable protein-protein interactions responsible for formation of the Ras-Raf complex

Cholic acid - a host for the long linear molecules

Co-crystals of cholic acid (CA) with n-alkylammonia (n=10, 12, 14, 16) are the first examples of CA's co-crystals with molecules of comparable size (Tomašić and Štefanić 2007). In one case a completely new type of bilayer arrangement was found. The host–guest ratio in crystals was 1:1 in three cases and 2:1 in one case. In 1:1 complexes CA molecules are assembled in bilayers and n-alkylammonia guests are included in the hydrophobic zones between those layers in a sandwich-type structure. In the 2:1 complex the CA bilayers form one-dimensional hydrophobic channels into which guest molecules are included. In the case of 1:1 co-crystals the bilayers of CA are separated much more than previously reported in order to accommodate large n-alkylammonia molecules. In spite of the different bilayer arrangements, the characteristic spacing in the plane of CA bilayers is remarkably similar to the majority of other known CA crystals.

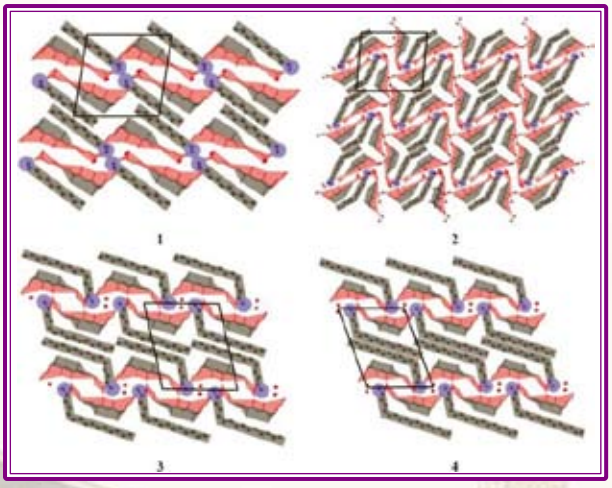

Figure 3: Bilayer arrangements of cholic acids in the crystal structures 1-4. The hydrophilic sides of cholic acids are shown in red, the NH^{3+} groups of alkylammonia in blue and hydrophobic regions in grey.

Coupled dipole-proton model on hydrogen-bonded ferroelectrics

Adiabatic approximations of a coupled dipole-proton model for hydrogen-bonded ferroelectrics show that models of interacting tunnelling protons and interacting dipoles which are employed for description of hydrogen-bonded ferroelectrics follow from the coupled dipole-proton model under the opposite adiabatic approximations and that the model of interacting dipoles seems to correspond better with the experiments (Merunaka and Rakvin 2007).

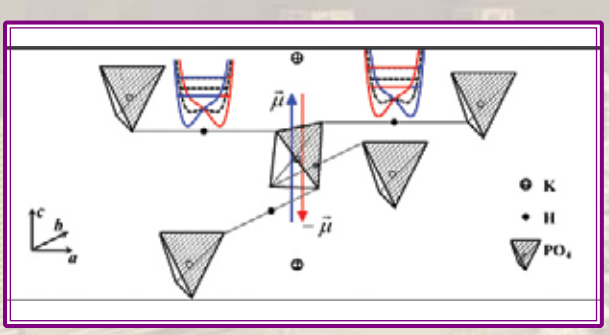

Figure 4: Structure of KH_2PO_4 and the coupled dipole-proton model. A double-well potential acts on the proton in O-H-O hydrogen bond. The dipole moment induced by deformation of neighbouring PO_4 group affects the hydrogen-bond potential due to dipole-proton coupling.

PATENTS

U.S. Pat. Appl. Publ. (2007) No. 11/672,789, Emmet M R, Kazazić S, Marshall A G, Greig M J: Analytical method for protein mapping using hydrogen/deuterium exchange.

NEW EQUIPMENT

The Divisional infrastructure was significantly improved by the acquisition of an X-ray diffractometer (Xcalibur Nova R), from Oxford Diffraction, financially supported by the Ministry of Science, Education and Sports. The new Xcalibur Nova R is an X-ray system designed for protein crystallography and applications where a high brilliance copper X-ray source is required. This is the first X-ray equipment in Croatian academic community suitable for a single crystal diffraction of biological macromolecules and this acquisition will enable new interdisciplinary research in the field of (bio)materials and life science.

Figure 5: X-ray diffractometer Xcalibur Nova R from Oxford Diffraction.

EDUCATIONAL ACTIVITIES

The Division provides 15 undergraduate and 15 graduate courses at Universities in Zagreb, Split, Rijeka, Osijek and Dubrovnik annually.

AWARDS

Leo Klasinc, Life Achievement Award for outstanding contributions in Natural Sciences awarded by the Croatian Parliament

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

1. Molecular structure and dynamics of systems with paramagnetic particles, Boris Rakvin
2. Surfactants, processes in solutions and at interfaces, Nada Filipović-Vinceković
3. Measurement and effect of atmospheric oxidants, Leo Klasinc
4. Advanced studies on chemical reactivity, Aleksandar Sabljić
5. Developing methods for modelling properties of bioactive molecules and proteins, Nenad Trinajstić
6. Design, synthesis and properties of organic ligands and their metal complexes, Ljerka Tušek-Božić
7. Protein-ligand interactions at atomic level, Marija Luić
8. Spectroscopy, chemical properties and reactions of biologically active molecules, Branka Kovač
9. Control of atomic and molecular dynamics by shaped electromagnetic fields, Nađa Došlić
10. Modeling molecules and materials by the mathematical and computational chemistry methods, Ante Graovac
11. Computational study of bio-macromolecules and development of new algorithms, Sanja Tomić
12. Development of mathematical methods for the description of molecular structure, dynamics and reactivity, Tomislav Živković
13. Amino-beta-lactams-synthrons for biologically interesting compounds, Ivan Habuš

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. Molecular structure, dynamics and reactivity, Boris Rakvin
2. Spectroscopy and modelling of bioactive molecules, Ante Graovac

Selected bilateral projects

1. Chemical applications of advanced ESR-techniques, Boris Rakvin (Bilateral project with Austria)
2. Combined experimental and theoretical study of structure and dynamics of hydrogen bonded systems, Nađa Došlić (Bilateral project with France, Program «COGITO»)
3. Ozone Pollution Index and National Air Quality Standard, Leo Klasinc (Bilateral project with China)
4. Applications of advanced Pulsed EPR techniques in the research of new fullerene-based materials: Structural properties of Li_4C_{60}, Boris Rakvin (Bilateral project with Slovenia)
5. Enzyme catalysis-model systems: Proton transfer in low barrier hydrogen bonds, Biserka Kojić-Prodić (Bilateral project with Slovenia)
6. Computer simulations of structure and dynamics of proteins, Sanja Tomić, (Bilateral project with Slovenia)
7. Novel bioflavonoids: (bio)chemical characterisation, structure/activity correlation and biotechnological application, Biserka Kojić-Prodić (Bilateral project with India)

Selected collaborative projects

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 physics P-15 action Advanced Para-

magnetic Resonance Methods in Molecular Biophysics, Boris Rakvin

SELECTED INVITED LECTURES

1. Kazazić S. Hydrogen/deuterium exchange reaction monitored by mass spectrometry: Probing higher order protein structure in 2nd Summer Course on Mass Spectrometry in Biotechnology and Medicine, Dubrovnik, Croatia, 7-15 July 2007.
2. Klasinc L. Oxygen, ozone, oxygen radicals - and life on Earth, Iowa State University, Ames, Iowa, USA, 05 March 2007.
3. Graovac A. Some novel results on topological indices. CHEMMOD 2007, The Babes-Bolyai University, Cluj-Napoca, Romania, 23-26 October 2007.

SELECTED ORGANIZED CONFERENCES

1. Final Evaluation Workshop of COST D 27 Action, Dubrovnik, 11-13 May 2007, organized by V Noethig-Laslo.
2. 22nd MATH/CHEM/COMP, Dubrovnik, 11-16 June 2007, organized jointly by A Graovac (ZFK) and D Plavšić, D Vikić-Topić, N Štambuk, P Konjevoda (NMR).
3. 2nd Opatija Meeting on Computational Solutions in the Life Sciences, Opatija, 4-9 September 2007, organized jointly by S Tomić, D Babić, and N Došlić (ZFK) and D Smith (ZOKB).
4. MMC 2007: Mathematical Methods in Chemistry. Split, 22-24 September 2007, organized by A Graovac.

SELECTED PUBLICATIONS

Chapters in books

1. Merunka D, Rakvin B. Anharmonic and quantum effects in KDP-type ferroelectrics: Modified strong dipole-proton coupling model. In: Ferro- and antiferroelectricity: Order/disorder cersus displacive. Dalal N, Bussmann-Holder A. (Eds). Springer Heidelberg-Berlin, 2007. pp 149-198.

Review articles

1. Amić D, Davidović-Amić D, Bešlo D, Rastija V, Lučić B, Trinajstić N. SAR and QSAR of the antioxidant activity of flavonoids. Curr Med Chem 2007: 14: 827.

Additional publications

1. Wenseleers W, Cambré S, Čulin J, Bouwen A, Goovaerts E. Effect of water filling on the electronic and vibrational resonances of carbon nanotubes: Characterizing tube opening by Raman spectroscopy. Adv Mater 2007: 19: 2274.
2. Marjanović M, Kralj M, Supek F, Frkanec L, Piantanida I, Šmuc T, Tušek-Božić Lj. Antitumor potential of crown ethers: structure activity relationships, cell cycle disturbances and cell death studies of a series of ionophores. J Med Chem 2007: 50: 1007.
3. Tomić S, Bertoša B, Wang T, Wade C. R. COMBINE analysis of the specificity of binding of Ras proteins to their effectors. Proteins 2007: 67: 435.
4. Tomasic A, Bertosa B, Tomic S, Soskic M, Magnus V. Binding behaviour of amino acid conjugates of indole-3-acetic acid to immobilized human serum albumin. J Chromatogr A 2007: 1154: 240.
5. Tomašić V, Štefanić Z. Cholic acid as host for long linear molecules: a series of co-crystals with n-alkylammonia. CrystEngComm 2007: 9: 1124.
6. Rožman M. Aspartic acid side chain effect - experimental and theoretical insight. J Am Soc Mass Spectrom 2007: 18: 121.
7. Merunaka D, Rakvin B. Adiabatic approximations of coupled dipole-proton model for hydrogen-bonded ferroelectrics. Phys Rev B 2007: 76: 140101.
8. Matanović I, Došlić N, Kühn O. Ground and asymmetric CO-stretch excited state tunneling splittings in the formic acid dimer. J Chem Phys 2007: 127: 014309.
9. Ljubic I, Sabljic A. Theoretical study of structure, vibrational frequencies, and electronic spectra of dibenzofuran and its polychlorinated derivatives. J Phys Chem A 2007: 111: 1339.

10. Došlić N, Kovačević G, Ljubić I. Signature of the conformational preferences of small peptides: A theoretical investigation. J Phys Chem A. 2007: 111: 8650.
11. Matasović B, Bonifačić M. Reductive halogen elimination from phenols by organic radicals in aqueous solutions. Chain reaction induced by proton-coupled electron transfer. J Phys Chem A. 2007: 111: 8622.
12. Novak I, Harrison LJ, Li W, Kovač B. Molecular and electronic structure of 1,8-peribridged naphthalenes. J Phys Chem A. 2007: 111: 2619.

Division of Organic Chemistry and Biochemistry

ZOKB

http://www.irb.hr/en/str/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, pep tide and glycopeptide chemistry, Štefica Horvat
- Laboratory for cellular biochemistry, Marija Abramić
- Laboratory for physical organic chemistry, Mirjana Eckert-Maksić
- Laboratory for molecular spectros copy, Goran Baranović
- Group for quantum organic chemistry, Borislav Kovačević

OVERVIEW OF THE DIVISION

From the beginning of 2007, scientists from the Division have been engaged in four research programs supported by Ministry of Science, Education and Sport, two of which are led by the members of the Division. The majority of the research groups are working on basic research in the fields of organic and bioorganic chemistry. The work in organic chemistry covers experimental and computational studies of molecular properties and reaction mechanisms, as well as the development of innovative synthetic methods and their application to the preparation of novel compounds for catalysis, host-guest chemistry and the pharmaceutical industry. Research in biochemistry is mainly focused on chemical transformations and structure-reactivity studies of different natural compounds in the context of improving the mechanistic understanding of important biological processes. Closely related, but more oriented toward medicinal chemistry, is a program focussed on the interaction of small molecules with DNA, RNA and proteins. Another important direction of research in Division encompasses projects related to development of new materials with emphasis on gel and supramolecular chemistry, liquid crystals and computational design of molecular wires. Finally, one research group, specialized in molecular enzymology, conducts its research within a program on bionanosystems and biocatalysis. The results of the work accomplished in the Division were published in 57 scientific papers, most of which appeared in renowned scientific journals. Two patent applications were also submitted.

As evidenced by the significant number of joint papers, the Division fosters intra- and extramural collaboration with most of the Croatian Universities and a number of research centres abroad. Members of the Division have made significant contributions to higher education by providing 12 courses at the under- and postgraduate levels and by supervising B. Sc. (4) and Ph.D (6) theses. They are also active in national and international societies and bodies and are involved in the editorial process of several international scientific journals, as editors, board members and referees. Last but not least, the Division participated in several projects with industrial companies from Croatia and from abroad.

TOP ACHIEVEMENTS

Reversible luminescent gels containing metal complexes

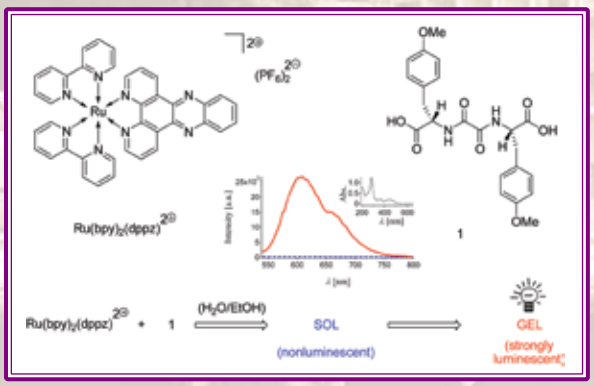

Figure 1. Luminescent gel formed by 1 and $Ru(bpy)_2(dppz)^{2+}$.

Evidence for the formation of luminescent gels in the presence of certain luminescent metal complexes was reported. Particularly interesting behaviour was exhibited by the $Ru(bpy)_2(dppz)^{2+}$ complex, which was found to be nonluminescent in the water/EtOH sol of gelator 1 (see Figure 1), while emitting when incorporated in the gel. This finding could constitute a basis for the luminescent probes in the monitoring of bond forming and breaking in soft materials (De Paoli et al., 2007).

Unusual self-organization in liquid crystalline dimers

The study of symmetric dimers comprising α,ω-diiminoalkylene flexible spacers revealed that the imino-linkage group plays a significant role in the generation of dipolar interactions favouring intercalated structures and, in conjunction with the spacer parity, strongly affects not only the geometry of the dimer but also the molecular arrangement within the smectic phase (Šepelj et al., 2007).

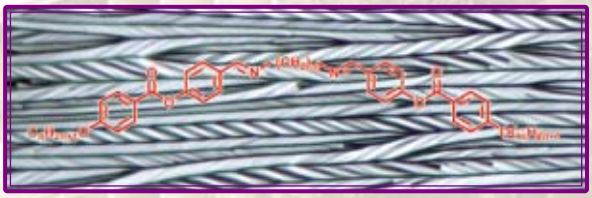

Figure 2. Texture of Nx phase.

New building blocks for molecular channels

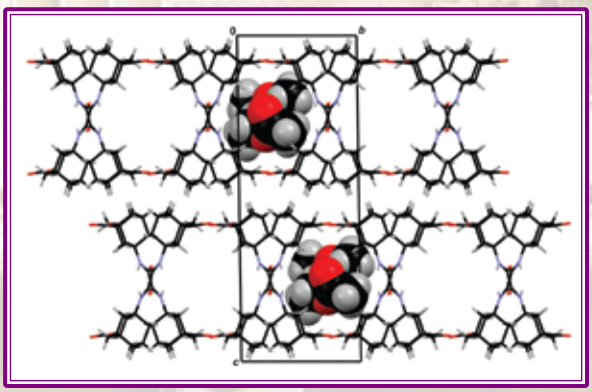

Figure 3. The crystal packing of 3·EtOAc with the two-dimensional hydrogen bonding network. Double layers parallel to (001) with solvent-filled channels running parallel to the direction [100] (Basarić et al., 2007).

Novel adamantane-oxalamide derivatives were prepared and structurally characterized. Interstingly, adamantane retropeptide, N,N'-bis(3-aminoadamantane-1-carboxylic acid)-oxalamide, showed a two-dimensional network with channels that can accommodate EtOAc molecules. This is the first example of such packing of oxalamides (Basarić et al., 2007).

Generation of chirality in solid state

A new example of the rare phenomenon of spontaneous generation of chirality was found for the conformationally chiral N-sulfonylpyrimidine derivatives. This compound forms two chiral conformations of M- and P-helicities and, upon crystallization, gives a conglomerate of enantiomorphous crystals, which showed mirror image solid-state CD spectra (Višnjevac et al., 2007).

Simulation of the photodeactivation of formamide in the n_O-π^* and π-π^* states

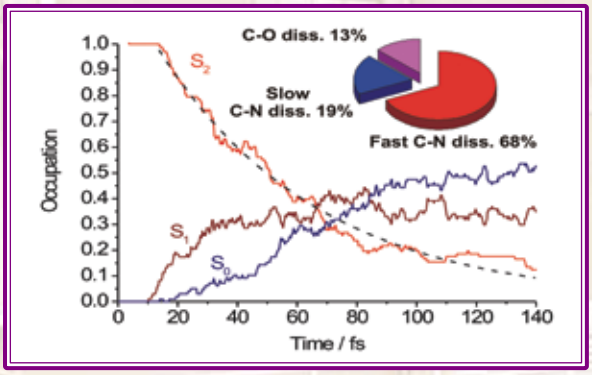

Figure 4 The fraction of trajectories for each state as a function of time and composition of photodeactivation paths, after excitation to the S_2 (π-π^*) state.

The short-time photodynamics (1ps) of formamide in its low lying singlet excited n_O-π^* and π-π^* states was investigated by the direct trajectory surface-hopping method. Simulations showed that, in both states, the primary deactivation process is C-N bond dissociation. In addition to the C-N dissociation pathway, C-O bond fission is found to be an additional primary deactivation path in the π-π^* dynamics. The paper describing this work (Antol et al., 2007) was selected for publication in the virtual Journals Series, which covers important results obtained by frontier research in cutting-edge fields.

Supramolecular superbases

It was shown that the supramolecule azacalix[3](2,6)pyridine is a hyperstrong neutral organic superbase, as evidenced by its proton affinity of 314.6 kcal mol^{-1} in the gas phase, and its associated pK_a value of 37.3 in acetonitrile. The reason behind this remarkable basicity was shown to be a very strong bifurcated hydrogen bond, reinforced by the cationic resonance effect (Despotović et al., 2007).

DNA and RNA studies

In vitro testing of novel styryl-2-benzimidazoles and benzimidazo [1,2-a]quinolines synthesized at the Faculty of Chemical Engineering and Technology, Zagreb, revealed pronounced antiprofilerative effects toward various human tumour cells and selectivity against certain tumours (Hranjec et al., 2007).

Understanding enzymatic reactivity with a computational approach

Glutamate mutase is a coenzyme B_{12}-dependent enzyme important in the metabolism of (S)-glutamate as well as in the biosynthetic pathways of various peptidyl antibiotics. Computational examinations shed light on its unusual inactivation in the presence of 2-thiolglutarate. In particular, an active-site glutamate was predicted to be responsible for the deprotonation of the thiol group and the subsequent generation of an extremely stable thioglycolyl radical (Sandala et al., 2007).

Human dipeptidyl peptidase III acts as a post-proline-cleaving enzyme on endomorphins

Based on the determination of affinity and hydrolytic activity towards several newly discovered opioid peptides, using capillary electrophoresis, it was found that dipeptidyl

peptidase III (DPPIII) accepts Pro (proline) at the P1 position of its substrate. This finding is in contrast to the accepted notion that proline imposes a restriction on the hydrolysis of the peptide bond that is catalysed by this type of enzyme (Baršun et al., 2007).

PATENT APPLICATIONS

Patent number P20070225A, Džolić Z, Žinić M, Cametti, M, Dalla Cort A, Mandolini L. Colorimetric sensors for detection of fluoride anion in solutions and gels. Patent number P20070111A, Basarić N, Renić M, Mlinarić-Majerski K. Adamantane-dipyrromethane compounds, method of preparation and applications in anion sensing. Both patents have been entered in the Patent Application Register, Patent Department, State Intellectual Property Office of the Republic of Croatia.

NEW EQUIPMENT

As part of a project funded within the Sixth Framework Programme and coordinated by David Smith, a new and powerful 56-processor computer cluster was purchased, assembled and installed in the Group for Quantum Organic Chemistry.

EDUCATION

The Division continued its involvement in educational activities in 2007 with 10 graduate courses and 2 undergraduate courses at the University of Zagreb. One graduate course was also held as part of the interdisciplinary Ph.D. study “Molecular Biosciences”, which is a joint initiative of the University J. J. Strossmayer in Osijek, the University of Dubrovnik, and the Ruđer Bošković Institute.

AWARDS

Robert Vianello was awarded the Leopold Ružička award for young scientists of the Croatian Chemical Society. Ina Nemet received a Postdoctoral Fellowship Award from the Juvenile Diabetes Research Foundation.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

1. Molecular enzymology and protein interactions of hydrolases, Marija Abramić
2. Macrocyclic ligands, structures in solutions and molecular spectroscopies, Goran Baranović
3. Organic and bioorganic processes in ground and excited states, Mirjana Eckert-Maksić
4. Chiral building blocks for biologically active molecules. Synthesis and reactivity, Zdenko Hameršak
5. Chemical transformations of natural compounds, Štefica Horvat
6. Cage compounds: Building blocks for molecular architecture, Kata Majerski
7. Brønsted and Lewis acids and bases in chemistry and biochemistry, Zvonimir Maksić
8. Policyclic structures with silicon, germanium and tin (valid until April 30), Davor Margetić
9. Study of interactions of novel compounds with biomacromolecules, Ivo Piantanida
10. Computational studies of protein structure and function, David Smith
11. Chiral organic materials - synthetic, structural and functional research, Vladimir Vinković
12. Synthesis of novel biologically active nucleobase and nucleotide derivatives, Biserka Žinić
13. Supramolecular chemistry of gels. Self-assembly approach to functional hybrid materials, Mladen Žinić

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. Design, synthesis and reactivity of (bio)organic molecular systems, Mirjana Eckert-Maksić
2. New small molecules targeting macromolecules of tumour and inflammatory processes, Ivo Piantanida

Research, developmental and international projects

1. Reinforcement of the Centre for Computational Solutions in the Life Sciences, David Smith (6th Framework Programme, EU-FP6-043749-ReCompSoLS)
2. Structure-function studies on metallopeptidases involved in metabolism of biologically active peptides, Marija Abramić (Bilateral Croatian-Austrian Project)
3. Modelling of Organic and Bioorganic Compounds and Processes in Ground and Excited States, Mirjana Eckert-Maksić (Bilateral Croatian-Austrian Project)
4. Protein engineering of halohydrin dehalogenases for the production of fine chemicals and pharmaceutical intermediates, Maja Majerić Elenkov (Croatian-Chinese bilateral project, 2007-2009)
5. Microheterogeneity in Aqueous Mixtures: An Investigation by Molecular Spectroscopy and Theoretical Methods, Goran Baranović (Croatian-French program "Cogito")
6. New functional dendritic materials: synthesis and self-organization, Andreja Lesac (Croatian-French program "Cogito")
7. Photochemical transformation of adamantane derivatives activated by phthalimides, Nikola Basarić (Bilateral project Croatia-Germany)
8. Experimental and Computational Study of Protonated Organic Molecules, Mirjana Eckert-Maksić (Bilateral project Croatia-Germany)
9. Computer-assisted Design of Strong and Ultrastrong Bases and their Applications, Zvonimir Maksić (Bilateral Croatian-German Project)
10. Metal-binding ability of Leu-enkephalin, related glycoconjugates and peptidomimetics: comparative CD and FTIR spectroscopic studies, Andreja Jakas (Bilateral Croatian-Hungarian project)
11. Pores and Channels by Assembly of Cyclic Peptides: Design, Molecular Modelling and Synthesis, Kata Majerski (Bilataral project Croatia-India)
12. Theoretical Study of Bioactive Molecules with Property of Releasing Nitrogen Monoxide (NO): N-nitrosohydroxylamine and its N- and O- alkyl Derivatives, Mirjana Eckert-Maksić (Bilateral Croatia-Slovenian project)
13. Theoretical and Experimental Investigations of the Intra- and Intermolecular Hydrogen Bonds, Zvonimir Maksić (Bilateral Croatian-Slovenian Project)
14. Intrinsic Properties of New Molecular Materials, project within COST D26 action; 2003-April 2007, Mirjana Eckert-Maksić
15. Thermally processed foods: possible health implication, Štefica Horvat and Andreja Jakas (COST 927, WG1 and WG5)
16. Transcription of bioinspired and designed functional modules into nanostructured smart gels, Mladen Žinić (COST D31, WG 20)
17. Synthesis of fluorescently-labelled macrolide probes, GlaxoSmithKline research centre Zagreb d.o.o., Zagreb, Kata Majerski
18. Synthesis and spectral analysis of new steroidal-haptens, TECNA s.r.l. Area di Ricerca, Padriciano, Trieste, Italy, Kata Majerski

SELECTED ORGANIZED CONFERENCES

1. The 2nd Opatija Meeting on Computational Solutions in the Life Sciences, Hotel Opatija, Opatija, Croatia, September 4-9, 2007, organized jointly by D Smith (ZOKB) and S Tomić, D Babić, and N Došlić (ZFK).
2. WG Meeting COST D31-0020-05 Transcription of Bioinspired and Designed Functional Modules into Nanostructured Smart Gels, September 30 to October 2 2007, organized by Z Džolić and M Žinić.
3. Computational modelling of properties and reactivity of molecules in the ground state and the excited states, Austrian-Croatian workshop, Institute "Ruđer Bošković", Zagreb, Croatia, November 6, 2007, organized by I Antol and M Eckert-Maksić.

SELECTED INVITED LECTURES

1. Žinić M. Supramolecular chemistry and stereochemistry of gel assemblies, University of Perugia, CEMIN, National Centre of Excellence for Innovative Nanostructural Materials for Chemical and Biochemical Applications, January 26, 2007.
2. Basarić N. Adamantane amino acd hydroxyl acids: incorporation into cyclic peptides and depsipeptides for the formation of new lipophilic tubular materials, Central Salt and Ma-

rine Chemicals Research Institute, Bhavnagar (Gujarat), India, May 9, 2007.
3. Basarić N. Pyrrole: the building block for chemical sensors, Central Salt and Marine Chemicals Research Institute, Bhavnagar (Gujarat), India, May 10, 2007.
4. Smith D. Theoretical studies of coenzyme B_{12}-dependent reactions: what can small models tell us, The Gordon Research Conference on Vitamin B12 and Corphins, University of New England, Biddeford, Maine, USA, July 1-6, 2007.
5. Margetić D, Warrener RN, Officer D, Butler DN, Dong Z, Merican Z, Hesheng T, Gunter MJ. Design and complexations of bis-porphyrin system aimed for light-harvesting devices, Novel Pi-systems, Novel Properties, Pre-symposium of the 12th International Symposium on Novel Aromatic Compounds (ISNA-12) Tokyo, Japan, July 21, 2007.
6. Margetić D, Butler DN, Warrener RN, Dong, Z, Merican Z, Officer D, Hesheng T, Gunter MJ. Molecular design, synthesis and complexation study of bis-porphyrin system aimed for light-harvesting devices, Functional Aromatic Compounds, Post-symposium of the 12th International Symposium on Novel Aromatic Compounds (ISNA-12), Harima, Japan July 30-31, 2007.
7. Vianello R, Maksić Z. Interpretation of the intrinsic molecular reactivity using triadic formula, The 2nd Opatija Meeting on Computational Solutions in the Life Sciences, Opatija, Croatia, September 4-9, 2007.
8. Maksić Z. MRCI calculations in organic chemistry, COST D37. GRIDCHEM Meeting, Rome, Italy, October 29-30, 2007.
9. Smith D. Theoretical studies of coenzyme B_{12}-dependent reactions: recent developments, The 1st Split Meeting on Development and Applications of Novel Methods and Models in Computational Biophysics and Structural Bioinformatics, Split, Croatia, December 19-21.

SELECTED PUBLICATIONS

1. Sandala G, Smith D, Marsh E, Radom L. Toward an improved understanding of the glutamate mutase system. J Am Chem Soc 2007: 129: 1623.
2. Crljen Ž, Baranović G. Unusual conductance of polyyne-based molecular wires. Phys Rev Lett 2007: 98: 116901.
3. De Paoli G, Džolić Z, Rizzo F, DeCola L, Vögtle F, Müller W.M., Richardt G, Žinić M. Reversible luminiscent gels containing metal complexes. Adv Funct Mater, 2007: 17: 821.
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12. Margetić D, Warrener RN, Sun G, Butler DN. The preparation of 7-substituted norbornadiene-2,3-dicarboxylic anhydrides and an experimental and theoretical study of their reactivity. Tetrahedron 2007: 63: 4338.
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Division of Materials Chemistry

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

ZKM

DIVISIONAL ORGANISATION

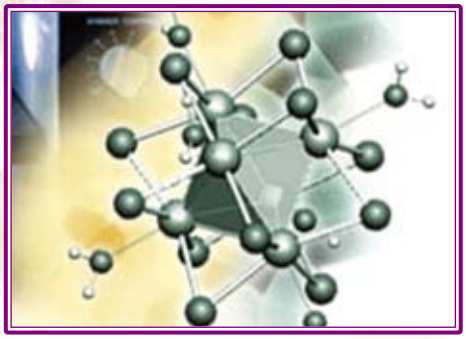
Head: Svetozar Musić

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

- Laboratory for synthesis of new materials, Boris Subotić
- Laboratory for precipitation processes, 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 ichtiopathology – biological materials, Rozelindra Čož-Rakovac

OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is a centre of excellence in materials science. We are strongly focused on the synthesis of various materials and the investigation of their chemical, microstructural, and physical properties. Our primary interests are in the areas of metal oxides, 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 handles all aspects of the physico-chemical effects of ionizing radiations and their applications. The low-dose and high-dose chemical dosimetry systems were developed and compared with different dosimeters produced in other countries. Our main research activities are financially sponsored by the Ministry of Science, Education and Sports. There are also numerous activities carried out in co-operation with sundry industries, hospitals, state institutions and faculties.



TOP ACHIEVEMENTS

Transformation of ferrihydrite to hematite in the solid state

Low crystalline ferrihydrite (2-XRD lines) was synthesized and characterized with ^{57}Fe Mössbauer spectroscopy from room temperature to 4.2 K, as well as in an external magnetic field. Upon heating of ferrihydrite to 493 K, Mössbauer spectra recorded at 78 and 12 K showed hyperfine-field distributions, presumably due to non-uniform chemical environments for the Fe^{3+} and/or to the shape and size distributions of hematite clusters. Ferrihydrite heated to 518 K showed a superposition of two sextets at 78 K. The outer sextet had Mössbauer parameters which indicated the coexistence of antiferromagnetic and weakly ferromagnetic

spin states in hematite. The much broader magnetic component was assigned to ferrihydrite. Upon heating of ferrihydrite to 598 K a well-crystallized hematite was produced (Ristić et al., 2007).

New oxalate-bridged ferromagnetically coupled $Cu^{II}Cu^{II}$ systems

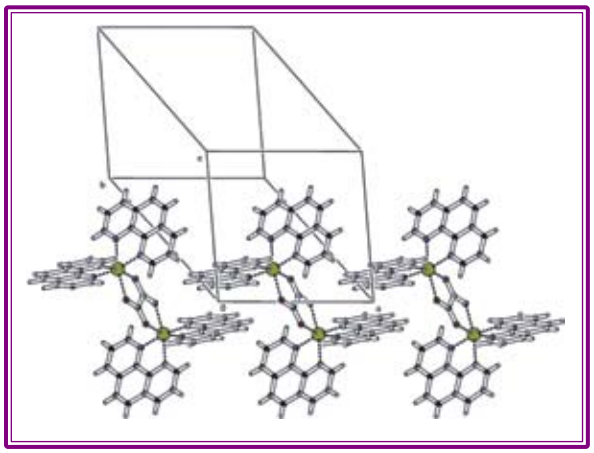


Figure 1. One-dimensional structural motif in 1 generated by the phenanthroline stacking interaction.

In the rational approaches to the design and synthesis of novel magnetic materials, the oxalate anion has often been used as a bridging ligand, since its rich binding facilities and abilities of mediating magnetic exchange interaction between metal centres could result in the formation of species with attractive new architectures and interesting magnetic properties.

The tris(oxalato)oxoniobate(V) anion, $[NbO(C_2O_4)_3]^{3-}$, has been used for the first time as the initial building block in the construction of polynuclear oxalate-bridged species. Two new compounds of the composition: $[\{Cu(phen)_2\}_2(\mu\text{-}C_2O_4)][Cu(phen)_2(\mu\text{-}C_2O_4)NbO(C_2O_4)_2]_2\cdot 8H_2O$ (1) and $[\{Cu(bpy)_2\}_2(\mu\text{-}C_2O_4)][Cu(bpy)_2(\mu\text{-}C_2O_4)NbO(C_2O_4)_2]_2\cdot 0.5bpy\cdot 7H_2O$ (2) (phen = 1,10-phenanthroline, bpy = 2,2'-bipyridine), with ferromagnetic exchange interaction within their dinuclear $Cu^{II}Cu^{II}$ units, have been prepared. In the crystal packing of both structures one-dimensional motifs dominate, generated by several types of ligand stacking interactions. The observed ferromagnetic interaction [with J = +5.9 cm^{-1} and +7.9 cm^{-1} for 1 and 2, respectively, (using $H_{INT} = -JS_1\cdot S_2$)] is the consequence of the suitable topology of the magnetic orbitals located on the copper(II) ions (Jurić et al., 2007).

Electronic structure of $LaFe_{12}B_6$, $DyCo_5$ and $TbCo_5$ intermetallics

The electronic structure of the intermetallic hydrogen-storage compounds $LaFe_{12}B_6$, $DyCo_5$ and $TbCo_5$ was studied with the aim of obtaining more information about their physical and chemical properties. The standard calculation methods within DFT (density functional theory) were used, whereby the corresponding approximations LSDA and LSDA+U (local spin density approximation) were employed. It was found that the calculated magnetic moments of $DyCo_5$ and $TbCo_5$ are in good agreement with experimental data (Miletić and Blažina, 2007). For the intermetallic compound $LaFe_{12}B_6$, low-moment and high-moment magnetic states were located, in agreement with experimental data. It was also found that the stability of the magnetic moment of Fe atoms depends on the kind of atoms surrounding Fe atoms within the unit cell. The stability of magnetic moment of Fe atoms at the 18(h) crystallographic site was found to be much more sensitive to its environment than the stability of magnetic moment of Fe atoms at 18(g) site.

Study of critical processes at zeolite crystallization

A population-balance analysis of the critical processes (nucleation, crystal growth) during the crystallization of zeolite A from a freshly prepared hydrogel and from the same freeze-dried hydrogel was performed. The analysis showed that the drastic treatment of hydrogel does not substantially change

either the distribution of nuclei in the matrix of the amorphous aluminosilicate precursor (gel), established during its precipitation, or the crystal size distribution of the crystalline end products (gel "memory effect") (Antonić Jelić et al., 2007). An equation of the gel "memory effect", which shows that crystal size distribution of the crystalline end product (zeolite) does not depend on either the hydrogel modification or crystallization conditions (for a constant number and distribution of nuclei in the gel matrix), was developed.

The applicability of positron lifetime (LT) spectroscopy to the study of the progress in the formation of secondary building units in aluminosilicate gel precursors yielding FAU and LTA type zeolites was investigated. Coexistence of the annihilation mode with long LT components was shown. A correlation between nucleation and type of exchanged ions was also indicated.

Preparation of solid phases with desirable morphological properties

A new method has been developed as a result of systematic investigations of the production of crystalline solid phases with the desirable physical-chemical properties. Calcium carbonate was chosen as an appropriate model system for such investigations being, at the same time, of great technological importance. It was successfully demonstrated that calcite crystals with different morphology characteristics can be produced in a chemical reactor, fully controlled by means of custom built electronics and software, by varying only process parameters, like temperature, supersaturation, gas mixture flow rate, stirring rate and mass concentration of reactants, rather than by additive addition (Ukrainczyk et al., 2007).

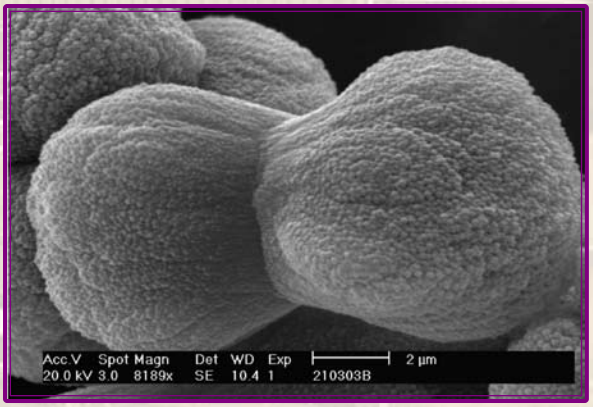


Figure 2. Calcite particles of high specific surface area.

Improvement of polypropylene composites as engineering plastics with elastomers

The effectiveness of different elastomers as impact modifiers and compatibilizers for polypropylene composites with different wollastonite fillers was studied by a comparison of structure-property relationships of polypropylene/wollastonite/elastomer composites and corresponding binary composites and blends. The composites modified with the poly(styrene-*b*-ethylene-*co*-butylene-*b*-styrene)-*g*-maleic anhydride (SEBS-g-MA) elastomer exhibited superior mechanical properties due to the excellent encapsulation ability of the polar SEBS-g-MA copolymer leading to more expressive core-shell morphology (Švab et al., 2007).

Advanced dosimetry methods

The response of the radiation accident personal chemical dosimetry system developed in the RCDL was systematically evaluated in different neutron fields. The response to neutrons was also calculated based on the LET (Linear Energy Transfer) distributions of monoenergetic neutrons. Very good agreement between the calculation and experiment was obtained, indicating to the predictive power of the calculation (Miljanić and Ražem, 2007).

The spectrum of dosimetry methods in use in the Radiation Chemistry and Do-

simetry Laboratory was extended to include phototransfered thermoluminescence (PTTL). The method was applied to dosimetry of ^{137}Cs gamma rays and neutrons of 14.5 MeV. The method allows for a separate determination of gamma and neutron component of the dose in mixed radiation fields (Miljanić et al., 2007).

Presence of unexpected phylogenetic lineages of brown trout (Salmo trutta L) in Gacka River, Croatia

Figure 3. Brown trout sampling for molecular and biochemical analyses.

The study provided the first analyses of mtDNA control-region variation of brown trout in order to assess their phylogenetic lineage affiliation and address the question of the origin of phylogenetic hyplotypes in the Gacka River. The prevalence of Danubian haplotype and no finding of Adriatic hyplotype imply an autochthonous status of the Danubian haplotype in Gacka River (Jadan et al., 2007).

The mission of the Ichtiopathology group is to become a well-recognized centre through scientific research in the ichthyohaematology, molecular ichthyology, and ichthyopathology fields, as well as establishing the Authorized Diagnostic Centre for Aquatic Organisms Diseases (ADD), which will perform diagnostic and specialized health surveys of fish, crustaceans and shellfish, through permanent education according to the EU demands and novel scientific information.

NEW EQUIPMENT

In 2007, the Laboratory for the synthesis of new materials received an Atomic absorption spectrophotometer Aanalyst-200 (Perkin-Elmer). In addition, an Ion Chromatography System, ICS-1000, Dionex Corporation was acquired.

EDUCATION

Scientists from the Division contributed to 9 undergraduate and postgraduate courses in 2007 as part of the involvement in the educational programs of Universities in Zagreb, Osijek and Dubrovnik. In addition, two PhD theses were successfully defended.

PATENTS

Patent number P20070240A. Kosanović C, Subotić B. Preparation for chemical treatment of sand-treated glass surfaces and hydrophobization of other glass, ceramic and rock surfaces.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

1. Synthesis and microstructure of metal oxides and oxide glasses, Svetozar Musić
2. Polynucelar metal systems – synthesis and properties, Pavica Planinić
3. Metal hydrides in clean energy systems, Želimir Blažina
4. Study of influence of aluminosilicate precursors on their transformations, Boris Subotić

5. Precipitation mechanism of inorganic biocompatible and related materials, Damir Kralj
6. Structure-property relationships of modified polymer materials, Ivan Šmit
7. Physico-chemical effects of ionizing radiations in materials, Dušan Ražem
8. Subcellular biochemical and phylogenetic diversity of aquatic organisms, Rozelindra Čož-Rakovac

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. New functional materials, Svetozar Musić

Other projects

1. Free Radicals in Chemical Biology (CHEMBIORADICAL), Branka Mihaljević, Project number: COST Action CM0603
2. Solid state dosimetry systems for various dosimetry fields, Maria Ranogajec-Komor, Bilateral scientific and technical co-operation between Croatian Academy of Sciences and Arts and Hungarian Academy of Science (2007 – 2009).
3. Characterization, intercomparison and application of radiophotoluminescence (RPL) dosimetry system according to international standards and protocols, Maria Ranogajec-Komor, Scientific co-operation between Ruđer Bošković Institute and Chiyoda Technol Corporation, Japan; Signed 18 July, 2007.
4. Radiation protection dosimetry in medicine, Maria Ranogajec-Komor and Saveta Miljanić, EURADOS Working Group 9 within Coordinated Network for Radiation Dosimetry (CONRAD) Project of the 6th Framework Programme of the EC; EURADOS coordinated project. (01.01.2005 – 31.12.2007).
5. Quality control methods and procedures for radiation technology, Dušan Ražem International Atomic Energy Agency Regional Technical Co-operation Project; Project number: RER 8/010
6. Nuclear techniques for the protection of the cultural heritage in the Mediterranean Region, Branka Katušin- Ražem; International Atomic Energy Agency Regional Technical Co-operation Project; Project number: RER 1/006
7. PHARE project: “Trout and Tourists”, Rozelindra Čož-Rakovac (department for Financing EU Assistance Programmes and Projects, Central Finance and Contracting Unit, 2005-0808-010101).
8. VIP project: “Model of revitalization and breeding of brown trout”, Rozelindra Čož-Rakovac (Ministry of Agriculture, Forestry and Water Management MAFWM, VI-1-10/05).
9. “Determination of genetic structure and restoration of autochthonous population of brown trout int he National Park Plitvice Lakes”, Rozelindra Čož-Rakovac (National Park Plitvice Lakes/Ministry of Environmental Protection, Physical Planning and Construction 21320/06).
10. Scientific/professional management of a project: “Breeding and Selection in Aquaculture”, Fishery 1961, Mato Hacmanjek (MAFWM, 324-01/06-01/202)
11. Scientific/professional management of a project: “Breeding and Selection in Aquaculture”, Fishery Vrnjika, Rozelindra Čož-Rakovac (MAFWM, 324-01/06-01/215)
12. Aquatic animal health monitoring – contracts with 8 international and national companies, Rozelindra Čož-Rakovac, Mato Hacmanjek.
13. Atomic force microscopy study of the crystallization of zeolite A, zeolite X and silicalite from amorphous (alumino)silicate, Cleo Kosanović (Croatian-Hungarian Intergovernmental S and T Cooperation Programme for 2007-2008).
14. Optimization of the synthesis process of zeolite A with special emphasis on the control of particulate properties (size and shape of zeolite A crystals), Boris Subotić (Bartex-Bartol and Ruđer Bošković Institute co-operation on scientific research).
15. Development of an adaptable technological procedure for the production of precipitated calcium carbonate, Damir Kralj (HITRA TP-01/0098-30)
16. The magnetic field influence on the calcium carbonate precipitation, Damir Kralj, bilateral Croatian-Slovenian cooperation.
17. Basic investigations of the mechanisms and kinetics of calcium carbonate polymorphs precipitation in artificial karst water, Damir Kralj (Hrvatske vode 325-01/07-02/63).

INVITED LECTURES

1. Miljanić S: TL and RPL detectors in mixed field dosimetry. Third International Workshop on Individual Monitoring, Oarai, Japan, December 3– 4, 2007.
2. Ranogajec-Komor M: Solid state dosimeters in environmental monitoring.Third International Workshop on Individual Monitoring, Oarai, Japan, December 3– 4, 2007.
3. Vekić B: Overview of EURADOS activities for individual monitoring.Third International Workshop on Individual Monitoring, Oarai, Japan, December 3– 4, 2007.
4. Katušin-Ražem B: Current status of food irradiation. Sixth Annual Meeting of Japanese Society of Radiation Safety Management, Tohoku University, Sendai, Japan, December 5 – 7, 2007.
5. Čož-Rakovac R: Presentation of Ichthyopathology Group-Biological Materials and Rudjer Boskovic Institute, 4th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 18, 2007.
6. Jadan M: Brown Trout in Neighbouring Countries, 4th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 18, 2007.
7. Hacmanjek M: Grayling in Croatia again? 4th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 18, 2007.
8. Strunjak-Perović I: Preservation measures for brown trout, 4th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 18, 2007.
9. Topić Popović N: Water Quality of Gacka River, 4th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 18, 2007.

ORGANIZED CONFERENCES

EURADOS CONRAD WG9 Meeting, Zagreb, 15 - 16 October 2007 (organized by S. Miljanić and M. Ranogajec-Komor). 14 scientists from 11 European countries were present.

SELECTED PUBLICATIONS

1. Ristić M, De Grave E, Musić S, Popović S, Orehovec Z. Transformation of low crystalline ferrihydrite to α-Fe_2O_3 in the solid state. J Mol Struct 2007: 834-836: 454.
2. Jurić M, Perić B, Brničević N, Planinić P, Pajić D, Zadro K, Giester G. Structure, stacking interactions and magnetism of compounds with oxalate-bridged dinuclear $Cu^{II}Cu^{II}$ and $Cu^{II}Nb^{V}$ units. Polyhedron 2007: 26: 659.
3. Miletić G, Blažina Ž. Magnetic properties of $DyCo_5$ and $TbCo_5$ intermetallics from the electronic structure calculations, J Solid State Chem, 2007: 180: 604.
4. Antonić Jelić T, Bronić J, Hadžija M, Subotić B, Marić I. Influence of the freeze-drying of hydrogel on the critical processes occurring during crystallization of zeolite A - A new evidence of the gel „memory" effect. Microporous and Mesoporous Materials 2007: 105: 65.
5. Ukrainczyk M, Kontrec J, Babić-Ivančić V, Brečević Lj, Kralj D. Experimental design approach to calcium carbonate precipitation in a semicontinuous process. Powder Technology 2007: 171: 192.
6. Švab I, Musil V, Šmit I, Makarovič M. Mechanical properties of wollastonite-reinforced polypropylene composites modified with SEBS and SEBS-g-MA elastomers. Polym Eng Sci 2007: 47: 1873. and Švab I, Musil V, Jurkin T, Šmit I. Phase structure and morphology of wollastonite-reinforced polypropylene composites modified with SEBS and SEBS-g-MA elastomers. Polym Eng Sci 2007: 47: 2145.
7. Miljanić S, Krpan K, Blagus S. TL and PTTL of TLD-100 and TLD-700 after irradiation with 14.5 MeV neutrons. Nuclear Instruments and Methods in Physics Research A, 2007: 574: 510.
8. Jadan M, Čož-Rakovac R, Topić Popović N, Strunjak-Perović I. Presence of unexpected phylogenetic lineages of brown trout Salmo trutta L. in Gacka River, Croatia. Aquac Res 2007: 38,15: 1682.

Division of Molecular Biology

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

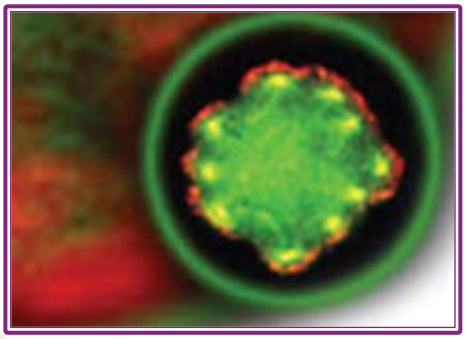
ZMB

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



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 and other fungi, cellular slime moulds, several invertebrates, plants and mammalian cells. The projects in our Division broadly comprise the following fields of study: maintenance of genome integrity and regulation of genome variation (DNA replication, recombination and repair); genome organization and repetitive DNA sequences; expression of genomic information (transcription and translation); signal transduction in molecular regulation of cell division, growth, differentiation and senescence; cellular responses to toxic agents and resistance to cytostatics and antibiotics; genetic background and regulatory mechanisms of neurotransmission; regulatory mechanisms of photosynthesis; physiology, biochemistry and structural biology of plant hormones; fungal biodiversity including taxonomy, biogeography and ecology of fungi; dynamical processes in the cytoskeleton; and 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 2007, members of the Division of molecular biology participated in the teaching of more than 30 undergraduate and postgraduate courses 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

Genomic phylostratigraphy

Macroevolutionary trends are traditionally studied by fossil analysis, comparative morphology or evo-devo approaches. With the availability of genome sequences and associated data from an increasing diversity of taxa, it is now possible to add an additional level of analysis: genomic phylostratigraphy. This is an innovative approach to understanding the origins of evolutionary novelties in the animal kingdom. As an example for this approach, a phylogenetic framework and embryo expression data from *Drosophila* was used to show that grouping genes by their phylogenetic origin can uncover footprints of important adaptive events in evolution (Domazet-Lošo et al., 2007).

Small GTPases from the marine sponge *Suberites domuncula*

Sponges (Porifera) are the simplest and the most ancient metazoan animals, which branched off first from the common ancestor of all multicellular animals. We have inspected ~13000 partial cDNA sequences (ESTs) from the marine sponge *Suberites domuncula* and have identified full or partial cDNA sequences coding for ~50 different Ras-like small GTPases. Small GTPases from sponge display a higher degree of sequence conservation with orthologues from vertebrates (53%–93% identity) than with those from either *Caenorhabditis elegans* or *Drosophila melanogaster*. Our results show that duplications and diversifications of genes encoding Ras-like small GTPases, especially the Rab subfamily of small GTPases, happened very early in the evolution of Metazoa (Četković et al., 2007).

Figure 1. Marine sponge Suberites domuncula in symbiosis with hermit crab.

Altered cell-cell adhesion in cisplatin-resistant human carcinoma cells

The development of cisplatin resistance in human laryngeal carcinoma cells was associated with an increase in β-catenin and a decrease in plakoglobin levels at cell-cell junctions. The observed alterations were an outcome of a slowly generating process, which was presumably a secondary event of the vital cellular response triggered by cisplatin toxicity (Čimbora-Zovko et al., 2007).

New fungal species

Figure 2. Basidiocarps of Conocybe thermophila, a new fungal species. It has been found on the island of Hvar and lives as a saprotroph of manured soil.

During research of Croatian fungal biodiversity, we found 466 fungal species of which 42 species and 4 genera were recorded as new to Croatian mycobiota, 1 species as new to European mycobiota, and 3 species were discovered as new to science. After *Scutellinia tuberculata* in 2000, *Gloiocephala cerkezii* and *Conocybe thermophila* are two fungal species discovered recently in our division (Hausknecht et al., 2007).

Figure 3. Basidiocarps of Gloiocephala cerkezii, a new fungal species. It has been found on two localities in the neighborhood of the city of Zagreb and lives as a saprotroph on plant remnants.

Protein-tyrosine phosphorylation and DNA replication in *Bacillus subtilis*

The *Bacillus subtilis* protein-tyrosine phosphorylation system PtkA/PtpZ is known to regulate the phosphorylation state of UDP-glucose dehydrogenases and single-stranded DNA binding proteins. Possible physiological effects of *ptkA* and *ptpZ* gene inactivation with respect to uronic acid content, competence, survival of gamma radiation-induced DNA lesions and DNA replication were investigated. The most striking phenotype observed was that of the Δ*ptkA* strain which exhibited an impaired cell cycle resulting in large cells with extra chromosomes that could be related to a defect in DNA replication (Petranović et al., 2007).

A new model for filopod protrusion

Cryo-electron tomography has been used to reconstruct, from filopodia of *Dictyostelium* cells, the 3-dimensional organization of actin filaments in connection with the plasma membrane. A special arrangement of short filaments converging toward the filopod's tip was discovered and termed a "terminal cone". Based on this finding a new model for filopod protrusion was proposed (Medalia et al., 2007).

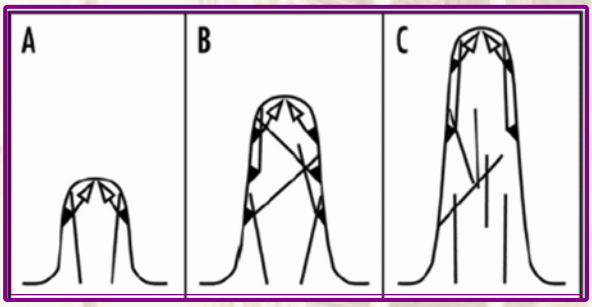


Figure 4. Model of actin organization in growing filopodia. This diagram illustrates the arrangement of actin filaments as revealed by cryo-electron tomography, in particular the conical arrangement of short filaments at the tip of filopodia in Dictyostelium cells.

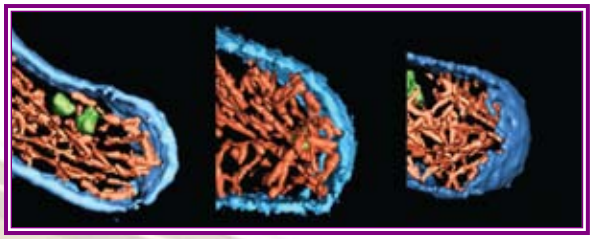


Figure 5. Three examples of the terminal cone, the arrangement of actin filaments at the tips of filopodia in *Dictyostelium* cells. In these reconstructions from cryo-electron tomography data actin is shown in red, and cell plasma membrane is shown in blue.

MODERN FACILITIES, METHODS AND EQUIPMENT

Centre for DNA sequencing

The DNA centre for DNA sequencing, under the supervision of Helena Ćetković as part of the Laboratory for Molecular Genetics, continued to provide services during 2007. Besides DNA sequence analyses, it also offers a microsatellite genotyping method for external users. More than 2500 sequence analyses were performed in this year at the DNA centre using ABI-Prism 3100 Sequencer.

Confocal laser scanning microscope

Confocal laser scanning microscope Leica TCS SP2 AOBS is equipped with eight laser excitation lines and four photomultiplier detectors. Instead of filters and dichroic mirrors, it uses acoustic-optical elements for spectral separation of fluorescence signals.

AWARDS

The esteemed National Science Award for scientific discovery in natural sciences was awarded to Ksenija Zahradka and Mirjana Petranović from our Division, together with Dea Slade and Miroslav Radman, for their research on genome repair and restoration by recombination under extreme conditions.

EDUCATION

Members of the Division of molecular biology teach over 10 undergraduate and over 20 postgraduate courses in biology, biochemistry, biophysics and biomedicine at the Universities in Zagreb, Dubrovnik and Osijek.

Figure 6. Cave-obligate sponge *Eunapius subterraneus* found in caves near the town of Ogulin, Croatia. (photo by I. Čukušić)

Figure 7. American blueberry plants (*Vaccinium corymbosum* L.) developed from cuttings upon plant hormone (auxin) treatment or regenerated by *in vitro* organogenesis (inset).

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

1. The role of recombination in DNA repair and genome evolution, Krunoslav Brčić-Kostić
2. Molecular mechanisms of DNA recombination and repair, Davor Zahradka
3. Fundamental molecular studies of Streptomyces biology, Dušica Vujaklija
4. Evolution and function of fast evolving portion of eukaryotic genome, Đurđica Ugarković
5. Evolution, properties and functional interactions of satellite DNA sequences, Miroslav Plohl
6. Transcriptional regulation in eukaryotes, Mary Sopta
7. Molecular mechanisms of imortalization and cellular aging, Ivica Rubelj
8. Cell response to cytotoxic agents and resistance development, Maja Osmak
9. Increase of adenovirus transduction efficacy and resistance to cytostatics, Andreja Ambriović Ristov
10. Serotonergic transmission: genes, proteins and behavior, Branimir Jernej
11. Serotonergic mechanisms in alcoholism, Lipa Čičin-Šain
12. Hydrodynamics of cerebrospinal fluid, Darko Orešković
13. Regulatory mechanisms of photosynthesis and differentiation of plastids, Hrvoje Fulgosi
14. Molecular regulation of plant development, Branka Salopek-Sondi
15. Genes and genomes: structures, functions and evolutions, Helena Ćetković
16. Molecular interactions in lymphocyte differentiation, Mariastefania Antica
17. Regulation of the cytoskeleton dynamics in cell motility and cytokinesis, Igor Weber

Program supported by the Ministry of Science, Education and Sports

1. Molecular fundaments of biological processes, Miroslav Plohl.

Other projects

1. 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)
2. Exploratory workshop on heterochromatin structure and function: from repetitive DNA sequences to epigenetics, Miroslav Plohl (European Science Foundation grant, ESF-EW 07-032)
3. Biophotonics approach to regulation of the actin cytoskeleton dynamics by small GTPase proteins, Igor Weber (UKF 1A Grant Agreement 9/07)
4. Engineering of GDSL-hydrolases and application of *Streptomyces* expression system, Dušica Vujaklija (MZOŠ, bilateral project with Austria, 911-02/05-06/35)
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. Adenovirus retargeting to aminopeptidase N and potential application in gene therapy of cystic fibrosis, Andreja Ambriović Ristov (MZOŠ, Cogito bilateral project with France, 910-08/06-01/00098).
7. Genetic diversity and evolutionary processes of irises along the Dinaric Alps, Hrvoje Fulgosi (MZOŠ, Cogito bilateral project with France, 910-08/04-01/0094)
8. Rho GTPases and adhesion mediated drug-resistance of tumor cells, Maja Osmak (MZOŠ, DAAD bilateral project with Germany, 911-02/05-04/09)
9. Dynamics of protein recruitment into a cortical complex, Igor Weber (MZOŠ, DAAD bilateral project with Germany, 911-02/05-04/11)
10. 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)
11. Plant hormones in development and biotic stress using biochemical and molecular approaches, Branka Salopek-Sondi (MZOŠ, bilateral project with Slovenia)

12. Synthesis and evaluation of new potential cytostatics from diazene family, Maja Osmak (MZOŠ, bilateral project with Slovenia, 910-08/05-01/00159)
13. Les plantes emblematiques commes indicateurs des processus microevolutifs dans les Balkans occidentaux, Hrvoje Fulgosi (ECO-NET 2007, trialateral project with France and Bosnia and Hercegovina)
14. Certified laboratory for the analysis of antioxidants in food products, Jasenka Piljac Žegarac (HITRA-TEST, E38-2005)
15. Development of methods for isolation and analysis of plant cellular components, Hrvoje Fulgosi (HITRA-TEST, E34/2006)
16. Regeneration of articular cartilage of the knee, Andreja Ambriović Ristov (MZOŠ, HITRA–TEST, 381-01/06-02/00032).
17. Propagation of the American highbush blueberry (*Vaccinium corymbosum* L.), Branka Salopek-Sondi (Center for agriculture at high altitudes, Primorsko-goranska county, applied collaborative project)
18. Propagation of aronia (*Aronia melanocarpa* L.), Branka Salopek-Sondi (Center for agriculture at high altitudes, Primorsko-goranska county, applied collaborative project)

SELECTED INVITED LECTURES

1. Plohl M, Mravinac B, Ugarković Đ, Durajlija-Žinić S: Organizational pattern of beetle satellite DNAs indicates high dynamics of recombinational events in centromeric heterochromatin. 16th International Chromosome Conference. Amsterdam, The Netherlands, August 25-29, 2007.
2. Čimbora-Zovko T, Fritz G, Osmak M: Lovastatin overcomes cisplatin resistance in human laryngeal carcinoma cells. 12th World Congress on Advances in Oncology and 10th International Symposium on Molecular Medicine. Hersonissos, Greece, October 11-13, 2007.
3. Ambriović Ristov A: Research Management Training Workshop (ReMaT). Zagreb, Croatia, November 5-6, 2007.
4. Zahradka K, Slade D, Bailone A, Sommer S, Averbeck D, Petranović M, Lindner A, Radman M: Survival of *Deinococcus radiodurans* in extreme conditions: genome restoration by recombination. Power of Microbes in Industry and Environment – Central European Symposium on Industrial Microbiology and Microbial Ecology. Zadar, Croatia, September 19-22, 2007.
5. Zahradka K: DNA repair in *Deinococcus radiodurans*: surviving extreme life conditions. MedILS Summer School 2007: Surviving death – an interdisciplinary approach workshop. Split, Croatia, July 29-August 4, 2007.
6. Ugarković Đ: Satellite DNA and centromere evolution. *Bio-Math Workshop* Mining and Meaning: Repetitive DNA in the Genomic Era. Leicester, United Kingdom, November 14, 2007.
7. Fulgosi H: The role of TROL protein in regulation of linear electron flow. Implications on nuclear gene expression. State Transitions Meeting. London, England, July 28-31, 2007.
8. Jernej B: Serotonergic synapse: from genes to behavior, Istituto superiore di sanita (Neuroscienze). Roma, Italy, April 20, 2007.
9. Jernej B: Development of original experimental rat model for serotonin research. University of Skopje. Skopje, Macedonia, May 3, 2007.
10. Weber I: Models and sensory limits in chemotaxis of eukaryotic cells. 2nd Opatija Meeting on Computational Solutions in the Life Sciences. Opatija, Croatia, September 4-9, 2007.

SELECTED ORGANIZED CONFERENCES

1. Summer school in applied molecular microbiology 2007. Split, Croatia, June 23 – July 1, 2007, Vujaklija D.
2. Third Croatian Neuroscience Congress (with international participation), Zagreb, Croatia, 2007, Jernej B.

SELECTED PUBLICATIONS

Research articles

1. Ćetković H, Mikoč A, Müller WE, Gamulin V. Ras-like small GTPases form a large family of proteins in the marine sponge *Suberites*

domuncula. J Mol Evol 2007: 64: 332.
2. Rass U, Ahel I, West SC. Actions of aprataxin in multiple DNA repair pathways. J Biol Chem 2007: 282: 9469.
3. Salopek-Sondi B, Vukelić B, Špoljarić J, Šimaga Š, Vujaklija D, Makarević J, Jajćanin N, Abramić M. Functional tyrosine residue in the active center of human dipeptidyl peptidase III. Biol Chem 2007: [Epub ahead of print].
4. Mravinac B., Plohl M. Satellite DNA junctions identify the potential origin of new repetitive elements in the beetle Tribolium madens. Gene 2007: 394: 45.
5. Zisowsky J, Koegel S, Leyers S, Devarakonda K, Kassack MU, Osmak M, Jaehde U. Relevance of drug uptake and efflux for cisplatin sensitvity of tumor cells. Biochem Pharmacol 2007: 73: 298.
6. Čimbora-Zovko T, Ambriović-Ristov A, Lončarek J, Osmak M. Altered cell-cell adhesion in cisplatin-resistant human carcinoma cells: A link between beta-catenin/plakoglobin ratio and cisplatin resistance. Eur J Pharmacol 2007: 558: 27.
7. Hausknecht A, Mešić A, Tkalčec Z. Two remarkable species of *Bolbitiaceae* (*Agaricales*) from Croatia. Österreichische Zeitschrift für Pilzkunde 2007: 16: 281.
8. Petranović D, Michelsen O, Zahradka K, Silva C, Petranović M, Jensen PR, Mijaković I. *Bacillus subtilis* strain deficient for the protein-tyrosine kinase PtkA exhibits impaired DNA replication. Mol Microbiol 2007: 63: 1797.
9. Domazet-Lošo T, Brajković J, Tautz D. A phylostratigraphy approach to uncover the genomic history of major adaptations in metazoan lineages. Trends in Genetics 2007: 23: 533.
10. Antica M**,** Dubravčić K, Weber I, Rajić LJ, Labar B, Batinić D. A quest for a mutation of the Aiolos phosphorylation domain in lymphocytes from leukemia patients. Haematologica 2007: 92: 260.
11. Medalia O, Beck M, Ecke M, Weber I, Neujahr R, Baumeister W, Gerisch G. Organization of actin networks in intact filopodia. Curr Biol 2007: 17: 79.

Invited review articles

1. Brozović A, Osmak M. Activation of mitogen-activated protein kinases by cisplatin and their role in cisplatin-resistance. Cancer Lett 2007: 251: 1.
2. Salopek-Sondi B, Magnus V. Developmental studies in the Christmas rose. International Journal of Plant Developmental Biology. 2007: 1: 151.
3. Gerisch G, Weber I. Toward the structure of dynamic membrane-anchored actin networks: An approach using cryo-electron tomography. Cell Adhesion & Migration. 2007: 1: 145.
4. Matulić M, Sopta M, Rubelj I. Telomere dynamics: the means to an end. Cell Proliferation. 2007: 40: 462.

Books

The book "Methods in molecular biology" published in November 2007 is the first manual of this kind in Croatian language. It introduces all basic methods of molecular biology, but also describes many specific techniques. The Editor-in-Chief Andreja Ambriović Ristov together with editors Anamaria Brozović, Branka Bruvo Mađarić, Helena Ćetković, Maja Herak Bosnar, Dubravka Hranilović, Silva Katušić Hećimović, Nevenka Meštrović Radan, Snježana Mihaljević, Neda Slade and Dušica Vujaklija gathered 119 authors from several institutions in Croatia. This book provides step-by-step protocols specifically designed for bench use. It also includes information about who-is-who in Croatia as far as particular experimental techniques are concerned, and thereby is hopefully going to promote collaboration among research groups in Croatia.

Figure 8. Editorial board of the multi-authored book "Methods in molecular biology".

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 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

Relevance of the granulocyte oxidative burst in host defence against cancer

The intensive oxidative burst of peripheral blood neutrophils of mice that were intramuscularly injected with melanoma B-6-F10 and/or subcutaneously with Sephadex G-200 was described for the first time to be important in host defence against cancer. Namely, the neutrophils from papula, developed at the site of Sephadex injection, were cytotoxic for the B16-F10 cells in vitro. However, the survival rate of Sephadex injected tumour-bearing mice was lower than that of the control animals bearing B16-F10, while their tumours grew faster and were less necrotic. Thus, it is likely that injection of Sephadex distracted the neutrophils from the tumour allowing faster progression of the tumour, indicating that neutrophils may have an important role in the host defence against malignant cells in the early stage of tumour development (Živković et al., 2007).

TOP ACHIEVEMENTS IN BASIC RESEARCH

Monoamine oxidase and dopamine beta-hydroxylase activity and polymorphisms

Increased platelet monoamine oxidase (MAO-B) activity with no effect of the MAO-B intron 13 polymorphism on platelet MAO-B activity (Pivac et al., 2007) was found in veterans with combat-related posttraumatic stress disorder. The same patients displayed decreased plasma dopamine beta-hydroxylase (DBH) activity and a similar frequency of the DBH genotypes (Mustapić et al., 2007).

Platelet serotonin in psychotic mania

Patients with bipolar affective disorder in a manic phase were found to have a higher platelet serotonin concentration than bipolar non-psychotic patients. This result suggests a biological distinction between the subtypes of bipolar affective disorder (Šagud et al., 2007).

p53 mutations in urothelial cancers from endemic nephropathy patients

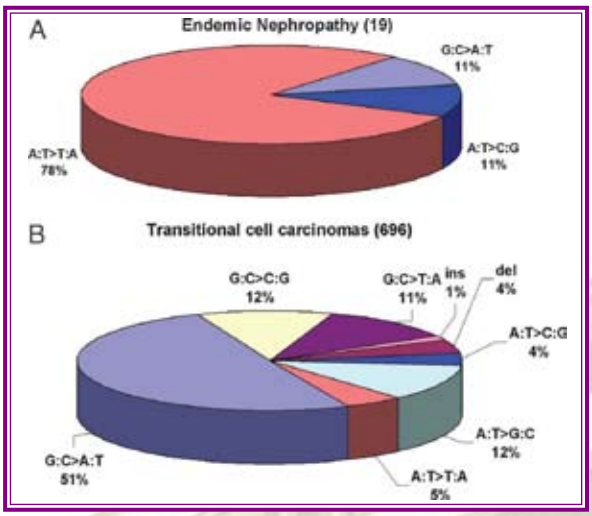


Figure 1. p53 mutational spectra in transitional cell carcinomas. (A) Transitional cell carcinomas from patients with EN. (B) Transitional cell carcinomas in kidney, renal pelvis, ureter, bladder, and unspecified urinary organs (data from the IARC p53 database).

Urothelial cancer tissues from upper urothelial tract of endemic nephropathy (EN) patients in Croatia were screened for p53 mutations. The immunohistochemically positively evaluated tumours were sequenced using Amplichip p53 Test (microarray assay) by Roche. Mutations of A:T pairs accounted for 89% of all mutations, with 78% being A:T→T:A transversions, the characteristic fingerprint observed in aristolochic-

acid-treated cells and animals. These data, together with characteristic DNA adducts lead to the conclusion that dietary exposure to aristolochic acid is a significant risk factor for EN (Grollman et al., 2007).

Functional analysis of human S-adenosylhomocysteine hydrolase

S-adenosylhomocysteine hydrolase (AdoHcyase) catalyzes the hydrolysis of AdoHcy to adenosine and homocysteine. Increased levels of AdoHcy may play a role in the development of cardiovascular diseases. Polymorphic isoforms named SAHH-1 to 4 exist in human and we have identified the genetic background of isoforms SAHH-1, SAHH-2 and SAHH-3 (Fumić et al., 2007).

TOP ACHIEVEMENTS IN APPLIED RESEARCH

Novel potential anticancer compounds

During 2007 over a hundred newly synthesized compounds were screened *in vitro* for potential anti-tumour activity and the possible mechanisms of action were ascertained for the most effective ones. Of special significance is the study that presents, for the first time, a systematic and interdisciplinary study on the potential anti-tumour ability (including cell cycle and cell death studies) and structure-activity relationships of 14 conventional crown ethers and their derivatives in vitro. We also computationally modelled the relationship of molecular structure to the biological activity of the tested crown ethers and evaluated the impact of various molecular descriptors on anti-proliferative ability of these compounds, shown in Fig. 2 (Marjanović et al, 2007).

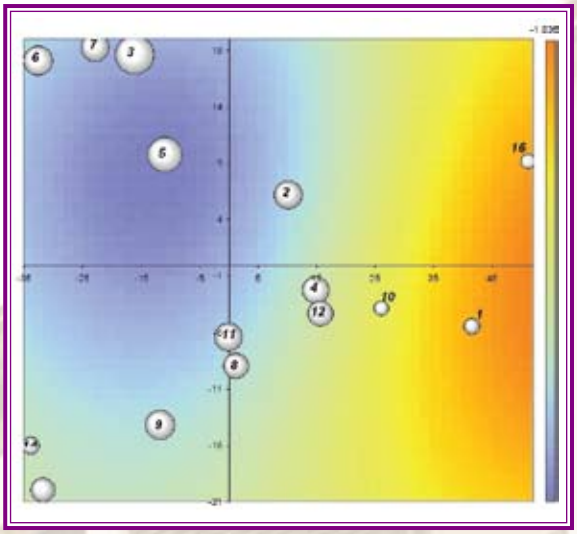


Figure 2. A heatmap visualization of the SVM regression model. Axes on the plot correspond to the first two principal components. Background colour illustrates the activity (as log IC_{50}), with more active in blue and less active in orange, predicted by the model. Radius of the disks is proportional to experimentally measured activity (as log IC_{50}) of each compound.

A novel therapeutic indication in psychotic PTSD

Treatment resistant psychotic PTSD, which is often complicated with suicidal attempts and lifetime functional impairment, was found to respond well to monotherapy with the atypical antipsychotic drug, quetiapine (Kozarić-Kovačić and Pivac, 2007).

Patents

Biodiesel fuel/fuel additive Oxidized Plant Oil Ethyl-ester Mixtures OPOEM - National patent pending, submitted by „Ruđer Bošković“ Institute, Franz Tatzber, Neven Žarković, Business and Administration Collage "Baltazar Adam Krečelić" and Milan Ermacora.

EDUCATION

A novel PhD study program, entitled „Biology of Cancer“, was jointly launched in 2007 by the Rudjer Boskovic Institute and the Universities of Split, Dubrovnik and Zadar. It is the first national PhD study programme with international evaluation and full ECTS accreditation. The first generation consists of 20 students, 16 of which originate from the Dubrovnik General Hospital. Neven Žarković was elected to act as the Vice- chair of the Study Council.

MODERN FACILITIES, METHODS AND EQUIPMENT

Novel Laboratory for Molecular Biosciences was established in Dubrovnik as joint research facility of the “Rudjer Boskovic” Institute, University of Dubrovnik and the Dubrovnik General Hospital. This is the first research laboratory in Dubrovnik that provides research facilities for the joint PhD studies, and will support networking within the B35 Action of COST and affiliated research networks.

Figure 3. A novel Laboratory for Molecular Biosciences in Dubrovnik.

AWARDS

National Award for the scientific achievements in the field of biomedicine

Award to Neven Žarković: The Croatian State Reward, the most prestigious scientific recognition available in Croatia, was given to Neven Žarković, senior scientist at the Division of Molecular Medicine, for the research in field of oxidative stress and oncology.

National Award for the Best Business Project

At the 10th National Economy and Entrepreneurship Forum in Šibenik, the project denoted "OxyLab", describing the development of the HNE-ELISA as a genuine analytical tool for oxidative stress, was presented by a team of students of the Project Management studies, joint studies of the Rudjer Boskovic Institute and the Business and Administration College "Baltazar Adam Krečelić". The project was recognized as the Best Business Project. The City of Zaprešić subsequently awarded the project team with the highest annual award for promotion of science.

INTERNATIONAL FUNCTIONS

European Molecular Biology Conference (EMBC) re-elected Krešimir Pavelić as a vice-president for the fourth time. Krešimir Pavelić is also a delegate of the Croatian Academy of Sciences and Arts in the European Science Foundation, a member of the Strategic Working Party of the EMBC, a member of the Standing Committee of the European Medical Research Council, a member of the Council of the European Molecular Biology Laboratory, and a president of the National Scientific Council of Croatia.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

1. Pharmacogenomics and proteomics of serotonergic and catecholaminergic system, Dorotea Muck-Šeler
2. Molecular basis and treatment of psychiatric and stress related disorders, Nela Pivac
3. Signal transduction in tumours: Hh-Gli interactions and therapeutic potential, Sonja Levanat
4. Molecular characterisation of S-adenosylhomocysteine deficiency in humans, Oliver Vugrek
5. New approaches in the treatment of malignant diseases, Marko Radačić
6. Stress, GABA-A receptors and mechanisms of action of neuropsychoactive drugs, Danka Peričić
7. Obtaining the structures like Langerhans islets from mouse stem cells, Mirko Hadžija
8. Gene therapy of tumours by modulating the molecules of immune system, Jasminka Pavelić
9. Role of membrane peptidases on tumour and normal cells, Jelka Gabrilovac
10. The mechanism(s) of cholesterol action in Alzheimer's disease, Silva Katušić Hećimović
11. Molecular genetics and pharmacogenetics of gastrointestinal tumours, Sanja Kapitanović
12. Aberrant DNA methylation in HPV associated lesions, Magdalena Grce
13. The role of different cell death responses to DNA-damage treatment, Marijeta Kralj
14. Epigenetic and Immunomodulatory Changes in Malignant Head and Neck Tumors, Koraljka Gall Trošelj
15. The role of nm23 genes in oral squamous cell carcinoma, Maja Herak Bosnar
16. The role of p53/p73 protein network in soft tissue sarcoma, Neda Slade
17. Immunopathogenesis of human recurrent herpes simplex virus infection, Zorica Mikloška
18. Lipids, free radicals and their second messengers in integrative oncology, Neven Žarković

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. Integrative genomics and proteomics in cancer research. Krešimir Pavelić
2. Pharmacogenomics, proteomics and psychophysiology of neuropsychiatric disorders, Dorotea Muck-Šeler

Research, developmental and international projects

1. Integrating and Strengthening Genomic Research in South East Europe (INTEGERS) FP7-REGPOT-2007-1 (Fran Borovečki, members of Coordination Committee: Dorotea Muck-Šeler, Nela Pivac)
2. Frontotemporal dementias and motor neuron disease (Rajka Liščić, Bilateral Cooperation with Slovenia; co-investigators: Dorotea Muck-Šeler, Nela Pivac)
3. Developing method for detection of inherited predisposition to breast cancer in Croatia. (Technological project 2005-2007, Ministry of Science and Technology, Republic of Croatia, Sonja Levanat)
4. Toxicological *in vivo* studies of Lectranal (MILSING Corp, Mirko Hadžija)
5. Hereditary Breast Cancer predisposition in Croatia and Hungary', (Croatian Hungarian Intergovernmental S&T Cooperation Programme 2007-2008, Sonja Levanat - Croatia, Edith Olah – Hungary)
6. The role of cholesterol in Alzheimer's disease (Alison Goate, NIH - Fogarty International Research Collaboration Award, USA, co-investigator: Silva Katušić Hećimović)
7. The mechanism(s) of cholesterol action in Alzheimer's disease (Silva Katušić Hećimović, Bilateral project with USA, co-investigator: Alison Goate)
8. Cellular sites of dual y-secretase cleavage (Silva Katušić Hećimović, Bilateral project with Germany, co-investigators: Harald Steiner, Sven Lammich)
9. p53/p73 network in chemoresistance. The relevance of dominant-negative p73 isoforms for chemosensitivity (Bilateral collaboration with Austria, Neda Slade)

10. The role of p73 in cell cycle control (Bilateral collaboration with France, Cogito, Neda Slade)
11. Development of vaccine agains herpes genitalis (Croatian Fond for development and employment, Zorka Mikloška)
12. 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
13. Effects of the lipid peroxidation product 4-hydroxynonenal on primary hepatocytes, (Croatian-Austrian Science Technology Cooperation Program, Neven Žarković)
14. Support of human bone growth in vitro by bioactive glass and 4-hydroxynonenal, (Austrian National Bank Jubileums Fond Research Grant, Renate Wildburger (LKH Graz) and Neven Žarković)
15. Novel, genuine assays for lipid peroxidation analyses in experimental oncology, (Bilateral project on scientific and technological research collaboration with France – COGITO, Neven Žarković)
16. Modifying drug resistance by oxidative stress and antioxidants (Bilateral Hungarian – Croatian Scientific and Technological Collaboration project, Neven Žarković)
17. Genetic testing of monogenetic diseases: cystic fibrosis, non-sindromic deafness, Rett syndrome, (Clinical Hospital Split, Children's Hospital Zagreb, Jasminka Pavelić)
18. Therapeutic effects of mushroom extracts, (HITRA, Mislav Jurin)
19. Development of drugs for treatment of Dupuytren disease (Croatian Fond for development and employment. Krešimir Pavelić).

SELECTED ORGANIZED CONFERENCES

1. Pivac N, Muck-Šeler D. Second Croatian Congress on the Stress Related Disorders: diagnostic procedures of the stress related disorders, Rabac, Croatia, May 3-5, 2007
2. Pivac N. 5th Croatian Congress of Pharmacology and 2nd Congress of Croatian Physiological Society with international participation, organizer of the symposium Neurobiological basis and treatment of posttraumatic stress disorders, Osijek, Croatia, September 19-22, 2007.
3. Grce M. The International Workshop on Human Papillomaviruses (HPV) and Consensus Recommendations for Cervical Cancer Prevention & Colposcopy Training, Cavtat, Croatia, April 18 - 20, 2007.

SELECTED LECTURES

1. Pivac N, Kozarić-Kovačić D, Grubišić-Ilić M, Mück-Šeler D. Neurobiology of psychotic PTSD. Cambridge/Luton International Conference on Mental Health 2007, Churchill College, University of Cambridge, Cambridge, United Kingdom, October 11-13, 2007.
2. Pivac N. Biological markers in Croatian veterans with increased suicidality. NATO advanced research workshop. Wounds of war: lowering suicide risk in returning troops. Hotel Amerika-Holzer, Klopeiner See, St Kantian, Austria, October 16-17, 2007.
3. Žarković N. 4-Hydroxynonenal – second messenger of free radicals. The Annual International Conference of the Romanian Society of Biochemistry and Molecular Biology, Timişoara, Romania, September 6-8, 2007
4. Žarković N. Potential Relevance of 4-Hydroxynonenal and Related "Second Toxic Messengers of Free Radicals" for Biomedical Effects of Some Nutraceuticals. Fourth International Conference on Mechanisms of Action of Nutraceuticals (ICMAN 4) The Science behind Nutraceuticals: Medical and Dietary Opportunities, Tel Aviv, Israel, October 21-24, 2007
5. Pavelić J. Animal rights versus animal welfare. In: 3. Sudosteuropaisches Bioethik-Forum, Mali Lošinj, Croatia, September 20-22. 2007.
6. Herak Bosnar M, de Gunzburg J, Bago R, Brečević Lj, Weber I, Pavelić J. NM23/NDPK Subunits in Head and Neck Tumour Cells: Where do they go? 12th World Congress on Advances in Oncology and 10th International Symposium of Molecular Medicine and Cancer Chemoprevention Symposium, Heraklion, Crete, Greece, October 11-13, 2007.

7. Herak Bosnar M, de Gunzburg J, Bago R, Weber I, Pavelić J, Perina D, Mikoč A, Ćetković H. Subcellular localization of NDPKs: How far is a sponge from a human? 7th International Congress of the NDP Kinase/NM23/ Awd Family, Dundee, United Kingdom, September 2-6, 2007.
8. Grce M. Introduction to the Cervical Cancer Prevention. ECCA symposium. Cervical Cancer Prevention - The Role of Patient Groups and Non-Governmental Organizations. Monte Carlo, Monaco, 3.10.2007.
9. Matovina M, Sabol I, Milutin Gašperov N, Grce M. HPV 16 DNA integration in precancerous cervical lesions. The 12th World Congress on Advances in Oncology, and 10th International Symposium on Molecular Medicine. Hersonisos, Crete, Greece, 11-13.10.2007.
10. Pavelic K. Recent highlights in molecular medicine. Joanneum Research Meeting. Graz, Austria, February 28, 2007.
11. Pavelić K. Casting Lights on Molecular Events Underlying Tumour Invasion and Metastasis: What can be Seen from the "Omics" point of View? Plenary lecture, 7th Slovenian Meeting of the Slovenian Biochemical Society with International Participation. Maribor, Slovenia, September 26-29, 2007.
12. Pavelic K. New achievements in molecular medicine. Rega Institute for Medical Research. Brussels, Belgium, June 1, 2007.

SELECTED PUBLICATIONS

1. Pivac N, Knežević J, Kozarić-Kovačić D, Deželjin M, Mustapić M, Rak D, Matijević T, Pavelić J, Muck-Šeler D. Monoamine oxidase (MAO) intron 13 polymorphism and platelet MAO-B activity in combat related posttraumatic stress disorder, J Affect Disord 2007: 103: 131.
2. Kozaric-Kovacic D, Pivac N. Quetiapine treatment in an open trial in combat related posttraumatic stress disorder with psychotic features, Int J Neuropsychopharmacology 2007: 10: 253.
3. Mustapić M, Pivac N, Kozarić-Kovačić D, Deželjin M, Cubells JF, Mück-Šeler D. Dopamine beta-hydroxylase (DBH) activity and -1021C/T polymorphism of *DBH* gene in combat-related posttraumatic stress disorder. Am J Med Genetics Part B Neuropsychiatry Genetics 2007: 144B: 1087.
4. Šagud M, Mihaljević-Peleš A, Pivac N, Jakovljević M, Mück-Šeler D. Platelet serotonin and serum lipids in psychotic mania. J Affect Disord 2007: 97: 247.
5. Marjanović M, Kralj M, Supek F, Frkanec L, Piantanida I, Šmuc T, Tušek-Božić Lj. Antitumor potential of crown ethers: structure activity relationships, cell cycle disturbances and cell death studies of a series of ionophores. J Med Chem 2007: 50: 1007.
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8. Hranjec M, Kralj M, Piantanida I, Sedić M, Šuman L, Pavelić K, Karminski-Zamola G. Novel Cyano- and Amidino-Substituted Derivatives of Styryl-2-Benzimidazoles and Benzimidazo[1, 2-a]quinolines. Synthesis, Photochemical Synthesis, DNA binding and Antitumor Evaluation. J Med Chem 2007: 50: 5696.
9. Grollman AP, Shibutani S, Moriya M, Miller F, Wu L, Moll U, Suzuki N, Fernandes A, Rosenquist T, Medverec Z, Jakovina K, Brdar B, Slade N, Turesky RJ, Goodenough AK, Rieger R, Vukelić M, Jelaković B. Aristolochic acid and the etiology of endemic (Balkan) nephropathy. Proc Natl Acad Sci USA 2007: 104: 12129.
10. Živković M, Poljak-Blaži M, Žarković K, Mihaljevic D, Joerg Schaur D, Žarković N. Oxidative burst of neutrophils against melanoma B16-F10. Cancer Letters 2007: 246: 100.
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Review articles

1. Pavelić J, Matijević T, Knežević J. Biological and physiological aspects of action of insulin-like growth factor peptide family. Ind J Med Res 2007: 125: 511.

Chapters in books

1. Kozaric-Kovacic D, Pivac N. Novel approaches to the diagnosis and treatment of posttraumatic stress disorder. In: The Integration and Menagement of Traumatized people after Terrorist Attack. NATO Security through Science series E: Human and Societal Dynamics – (S. Begec, ed), vol 15 . IOS Press Amsterdam 2007. pp 13-40.
2. Pivac N, Kozarić-Kovačić D, Deželjin M, Mustapić M, Jovanović T, Mück-Šeler D. Neurobiology of Posttraumatic Stress Disorder. In: The Integration and Menagement of Traumatized people after Terrorist Attack. NATO Security through Science series E: Human and Societal Dynamics – (S. Begec, ed), vol 15. IOS Press Amsterdam 2007: pp 41-62.
3. Pivac N, Kozarić-Kovačić D, Mustapić M, Deželjin M, Nenadić-Šviglin K, Muck-Šeler D. New research on alcohol abuse and alcoholism (Peripheral biological markers in alcoholism) Chapter I. In: Drug and Alcohol abuse Research Focus. (Walcott, Terry A, ed). New York 2007, Nova Publishers, pp 1-62

Books

Methods in molecular biology /Metode u molekularnoj biologiji (Ambriović Ristov A, Brozović A, Bruvo Mađarić B, Ćetković H, Herak Bosnar M., Hranilović D, Katušić Hećimović S, Meštrović Radan N, Mihaljević S, Slade N, Vujaklija D, eds). Rudjer Boskovic Institute, Zagreb 2007.

Division of Marine and Environmental Research

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

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 DIVISION

During 2007, division scientists worked on more than 60 research projects contracted by the Ministry of Science, Sport and Education and outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from satellite oceanography down to nanotechnology. Each project contributed to the overall mission of the division, which is to strive for excellence in fundamental and applied research of environmental systems, their processes, states and control. The research is directed toward an increase in the knowledge base needed for the optimum management of the environment and hence to the benefit of our country and, indeed, the whole world.

The research results were published in 49 scientific papers in journals indexed by Current Contents. In addition, one patent was filed, three books were published, 17 invited lectures were held and 9 conferences were

organized. Also 4 graduate school studies were coordinated, and 2 B.Sc, 1 M.Sc. and 2 Ph.D theses were defended, under the mentorship of Division scientists. Finally, 12 undergraduate and 53 post-graduate courses were given at universities in Croatia and abroad.

TOP ACHIEVEMENTS

Modelling the northern Adriatic double-gyre response to intense bora wind: A revisit

A combination of recent intensive observations and simulations with two numerical models was used to address the issue of the northern Adriatic response to strong bora episodes. New observed and simulated data reinforced the view that an episode of strong bora wind provoked a double-gyre response north of the Po Delta - Pula line (Kuzmić et al., 2007).

Overfishing of anchovy (*Engraulis encrasicolus, L.)* in the Adriatic Sea

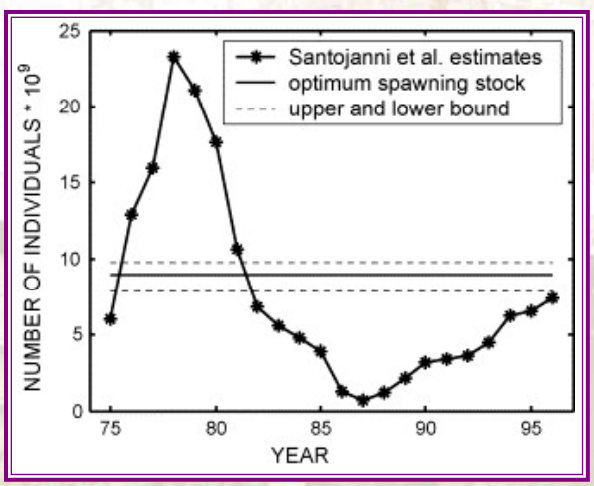


Figure 1. Stock of anchovy in the Adriatic Sea

Based on the analysis of published data series of anchovy stock size estimates for the period from 1975 to 1996, the stage dependent model was constructed. It was found that the anchovy population is below the optimum level, i.e. overfished since 1982. Evidence of overfishing was found in 1982, 1985, 1986 and 1988 (Klanjšček and Legović, 2007).

New three-dimensional particle tracking model for prediction of benthic carbon loading beneath fish farms

A model is based on stochastic differential equations for particle transport consistent with the well-known semi-empirical advection-diffusion equation. The model was applied to predict benthic carbon loading beneath fish farms. It requires only input data that is easily obtainable, in the form of measured current record, source and a specification of local bathymetry. The model accounted for advection by long-term residual and tidal currents, turbulent diffusion, realistic bathymetry and variations in daily (monthly, yearly) emissions from fish farms (Jusup et al., 2007).

Detection and functional characterization of efflux transporters in fish hepatoma cell line

The fish PLHC-1 hepatoma cells derived from topminnow (*Poeciliopsis lucida*), the most frequently used fish cell line in aquatic toxicology, expressed toxicologically relevant ABC efflux transporters involved in detoxification and excretion of xenobiotics (phase III). Moreover, the fact that the PLHC-1 cells possed all three critical elements of cellular detoxification machinery (phase I, II and III) additionally affirmed this cell line as a reliable and useful *in vitro* model in (eco)toxicological research (Žaja et al., 2007).

Chronic accumulation of cadmium in fish liver cytosol (Mullus barbatus)

Cytosolic metal concentrations in the liver, kidney and intestine decrease as follows: Fe≈Zn>Cu>Mn>Cd. In the liver cytosol association of MT and metals that induce MT synthesis was evident for Zn and Cu, but not for Cd. Cadmium concentration in the liver cytosol was an excellent marker of chronic accumulation of Cd with fish age ($r=0.69$, $p<0.01$) (Filipović Marijić and Raspor, 2007).

Seasonal dependence of metal concentrations in the chub gill cytosol

The correlation between the cytosolic metal and protein levels in the gills of chub, caught in the Sava River over two seasons, was examined. In specimens caught in the autumn, a positive correlation was obtained between the gill mass and the total cytosolic protein, Mn, Zn and Fe concentrations. In the spring, negative or low correlation of these parameters with the chub gill mass was observed (Dragun et al., 2007).

New methods for determination of xenobiotic chemicals and their application in field and laboratory experiments

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, several persistent intermediates from vitamin C production, and polycyclic aromatic hydrocarbons and their hydroxylated metabolites (Grung et al., 2007). The methods were applied to the determination of these contaminants in different environmental matrices (wastewater, river water, ground water, fish).

Pollution of electrochemical laboratory by gaseous mercury

A concentration of total gaseous mercury was measured in the atmosphere of an electrochemical laboratory using the CV AAS technique. By permanent aeration of laboratories the concentration of total gaseous mercury can be decreased almost ten times. In the open air of the electrochemical laboratory in Šibenik, the concentrations of total gaseous mercury during a long duration of the Bura wind are as low as the concentrations in the polar region i.e. between 0.6 and 1.8 ng/m^3 (Kwokal et al., 2007).

Barium in the Kupa river

Using a combination of geochemical and medical methods, an investigation was started on the possible impact of waste disposal on human health in Lokve, where about 18% of the total inhabitants have serious medical problems (Frančišković-Bilinski et al., 2007).

Metal sulfide nanoparticles in model solutions and natural waters

Growing evidence suggests that metal sulfide nanoparticles of natural origin exist in aquatic environments, even in the presence of dissolved oxygen. It was shown that metal sulfide nanoparticles readily adsorb and concentrate at a mercury electrode surface. Nanoparticles in two meromictic lakes were measured and an experimental procedure to clarify the nature of particles was proposed (Bura-Nakić et al., 2007).

Organic matter in Arctic and Barents Sea

Characterization of hydrophobic/hydrophilic properties of the organic matter in the northern Barents Sea shelf region and eastern Arctic Ocean revealed the dominance of more hydrophobic substances in the upper mixed layer and highly hydrophilic substances in deep waters (Gašparović et al., 2007).

Characterization of surface active substances in rainwater

Surface active substances as organic constituents of bulk precipitation were studied by the AC voltammetric method. The adsorption characteristics at the mercury electrode of real rainwater samples were compared with those of aqueous solutions of a number of model substances, which have been suggested to be representative of water soluble organic compounds in atmospheric aerosols and droplets (Ćosović et al., 2007).

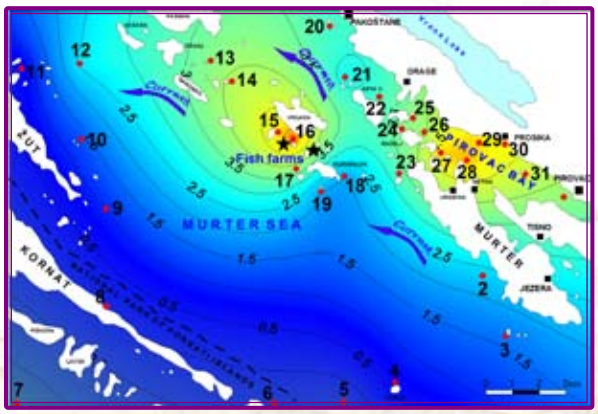


Figure 2. Spatial distribution pattern of $\delta^{15}N$ values in marine sponge Aplysina aerophoba during May 2005 around fish farms in Pirovac Bay and the Murter Sea (Central Adriatic), Kniewald G.

Geochemical map of $\delta^{15}N$ values in organic matter and organisms in coastal waters

The effect of fish-farm- and sewage-derived particulate nitrogen in the Murter Sea and semi-enclosed Pirovac Bay (Central Adriatic, Croatia) was assessed using the stable nitrogen isotopic composition ($\delta^{15}N$) in particulate organic matter (POM) and benthic sessile invertebrates (Dolenec et al., 2007).

PATENT

WO 2007/0966681 A1. Hršak D, Havriluk M. Mixed bacterial culture for atrazine degradation.

New equipment

The Iatroscan MK-6 is thin layer chromatograph measuring samples by means of a Flame Ionization Detector (FID) and a Flame Photometric Detector (FPD). The instrument is used for analysis and separation of lipid classes from nonpolar lipids such as hydrocarbons and polar phospholipids (Gašparović B.)

EDUCATION

Four graduate school studies were coordinated by the Division members. This includes studies on Biophysics with the University of Split, on Environmental Management and Oceanography with the University of Zagreb, and Environmental Protection and Nature Conservation with the University J.J. Strossmayer in Osijek. Twelve undergraduate and fifty three post-graduate courses were given at universities in Croatia and abroad.

HONOURS AND AWARDS

Legović T. Secretary General, International Society for Ecological Modelling (ISEM), 2007.

Lulić S. Acknowledgment for the exceptional contribution to nuclear safety. State department for nuclear safety, Zagreb, 2007.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

1. Organic compounds as molecular markers of anthropogenic impact to the environment, Marijan Ahel
2. Radionuclides and trace elements in environmental systems, Delko Barišić
3. Electroactive films for ecologicaly acceptable

conversion and energy storage, Višnja Horvat- Radošević
4. Biogeochemistry of metals in sedimentary systems and soils in Croatia, Goran Kniewald
5. Nature of organic matter, interactions with microconstituents and surfaces in the environment, Zlatica Kozarac
6. Mathematical modelling of circulation and remote sensing of boundary processes, Milivoj Kuzmić
7. Ecological modelling for sustainable management of resources, Tarzan Legović
8. Elektroanalitical research of microcrystals and traces in dissolved subtances, Milivoj Lovrić
9. Interactions of trace metal species in aquatic environment, Ivanka Pižeta
10. Metal-induced cellular changes in aquatic organisms, Biserka Raspor
11. Information systems on environmental quality and risk, Ivica Ružić
12. Multixenobiotic resistence mechanism as a biomarker of environmental quality, Tvrtko Smital
13. Nanoparticles in biogeochemical processes in the environment, Ivan Sondi
14. Surface forces on atomic scale applied in marine science and nanotechnology, Vesna Svetličić
15. Pathology of aquatic organisms in relation to pollution and aquaculture, Emin Teskeredžić
16. Networked Economy, Z. Skočir and Jadranka Pečar-Ilić

Program supported by the Ministry of Science, Education and Sports

1. Biogeochemical processes and environmental risk, Marijan Ahel

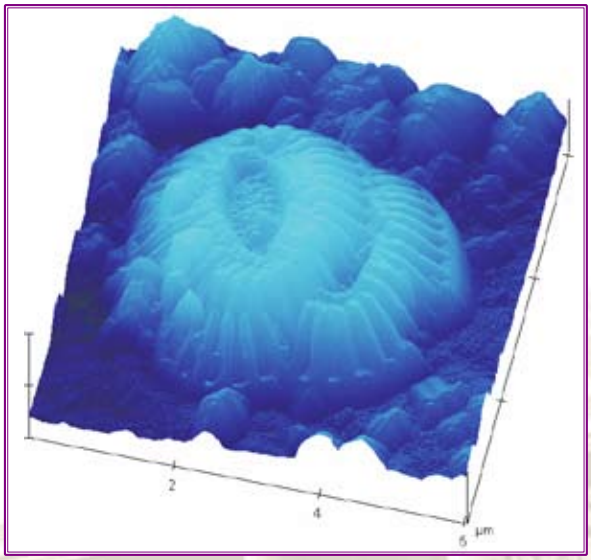


Figure 3. Marine Coccolithophor possibly Emiliania huxley from Adriatic seawater sample imaged by AFM. 3D image size 6 µm x 6 µm x 550 nm. (Mišić T., Svetličić V. and Hozić Zimmermann A.)

Selected international projects

1. Sava River Basin: Sustainable use, management and protection of resources, Biserka Raspor (EU FP6)
2. Reduction of environmental risks, posed by emerging contaminants, through advanced treatment of municipal and industrial wastes, Marijan Ahel (EU-FP6)
3. Ecosystem Approach for Sustainable Aquaculture, Tarzan Legović (EU-FP6)
4. Assessment of hazardous chemical contamination in the Sava River basin, Marijan Ahel and Tvrtko Smital (NATO Science for Piece)
5. Mechanism of mucilage formation in the Northern Adriatic Sea, Vera Žutić (Bilateral Cooperation with NSF, USA, Scripps Institution of Oceanography)
6. Novel physical chemical techniques to characterize the sea surface microlayer, Zlatica Kozarac (UK Royal Society)
7. Marine science and coastal management in the Adriatic Western Balkan, An education and research network, Božena Ćosović (Norwegian cooperation programme on research and higher education)

8. Electrochemical characterization of marine polysaccharides, Marta Plavšić (Deutsche Forschungsgemeinschaft)
9. Evaluation of contamination of stream sediments in lithologically different drainage basins, using advanced geomathematical methods, Stanislav Frančišković-Bilinski (Austrian-Croatian bilateral cooperation)
10. Multidisciplinary investigations of stream water sediments, soil and model compounds, that point to the clean and polluted environment, Halka Bilinski (Hungarian-Croatian bilateral cooperation)
11. Characterization of river sediment contamination from humid tropical Hugli River, India and temperate rivers of Croatia in terms of geochemical and mineralogical data based on weathering, Halka Bilinski (Indian-Croatian bilateral cooperation)
12. AFM study of the crystallization of synthesized zeolites, Vesna Svetličić (Bilateral Cooperation project with Eötvös Loránd University, Budapest, Hungary)
13. Biogeochemical processes in anoxic environments: electrochemistry as an alternative tool for trace metals and sulfur determination, Irena Ciglenečki-Jušić (Bilateral collaboration with Eötvös Loránd University, Budapest, Hungary)
14. Impact of fish farms on marine ecosystems of the Adriatic Sea, Goran Kniewald (Croatian-Slovenian bilateral cooperation)
15. Radiological monitoring around Nuclear Power Plant Krško, Slovenia, Stipe Lulić.

SELECTED ORGANIZED CONFERENCES

1. 6th European ecological modelling conference, Trieste, Italy, 27-30 November 2007, T Legović
2. Regional Biophysics Conference, Balatonfüred, Hungary, 21- 25 August, 2007, V Svetličić
3. Goldschmidt Conference on Geochemistry, 19-24 August, Köln, Germany, 2007, I Ciglenečki-Jušić
4. Workshop and International mezocosmos experiment "Phosphorus Limited Carbon Fixation, Cycling and Persistence and Role of Aggregation in the Processes", Piran, Slovenia, 16-22 October 2007, V Žutić
5. 10th Reunion of the Laboratories accredited for water analysis, Poreč, Croatia, October 23-26, 2007. B Raspor
6. 4th Croatian Conference on water with international participation: "Croatian water and European Union-chalenges and possibilities", Opatija, Croatia, 17-19.05.2007, Z Kozarac.

SELECTED INVITED LECTURES

1. Ahel M., Terzić S. Persistent intermediates from vitamin C production: Analysis, behavior and possible environmental implications , ACS meeting, Symposium honouring Walter Giger, Boston, USA, August 2007.
2. Barišić D. Research of locations with increased content of naturally occurring radioactive materials: Examples from Croatia. Naturally Occuring Radioactive Materials (NORM): Harmonization of Environmental Monitoring Methodologies, Sarajevo, Bosnia and Herzegovina, June 18-22. 2007.
3. Jusup M, Klanjšček J, and Legović T. Modelling deposition of particulate organic waste underneath aquaculture facilities: Validation of KK3D model, The sixth European ecological modelling conference, Trieste, Italy, 27-30 November 2007.
4. Klanjšček T, Nisbet R M, Neubert G, and Caswell H. When things are tough, they get even worse: the negative synergy of maternal transfer, bioaccumulation, exposure and low food availability. 17th Biennial Conf. On Biology of Marine Mammals, Cape Town, S. Africa, 29 Nov.- 3 Dec., 2007.
5. Kniewald G. Evidence of mantle source volcanism in the Adriatic region. International Conference on Evolution, Transfer and Release of Magmas and Volcanic Gases, Taipei, Republic of China, 22-27 April 2007.
6. Kniewald G. Geochemical alteration of gastropod shells from cretaceous carbonates impacted by lateritization – Donje Orešje, Croatia, 18th International Symposium on Environmental Biogeochemistry, Taupo, New Zealand, 11-17 November 2007.
7. Legović T. Future of marine resource management, The sixth European ecological modelling conference, Trieste, Italy, 27-30 November 2007.

8. Mihelčić G. Medical geology. Croatian Academy of Sciences and Arts, Zagreb, October, 2007.
9. Smital T. Ecotoxicological Relevance of the ABC Transport Proteins in Aquatic Organisms - from multidrug (MDR) to multixenobiotic (MXR) resistance and back. CIIMAR, University of Porto, Porto, Portugal, June 26-27, 2007.
10. Raspor B. Interpretation of natural fluctuations of metallothioneins and metal levels in the aquatic organisms. 35th Congress of the International Society for Oncodevelopmental Biology and Medicine, Prague, Czech Republic, September 16-19, 2007.

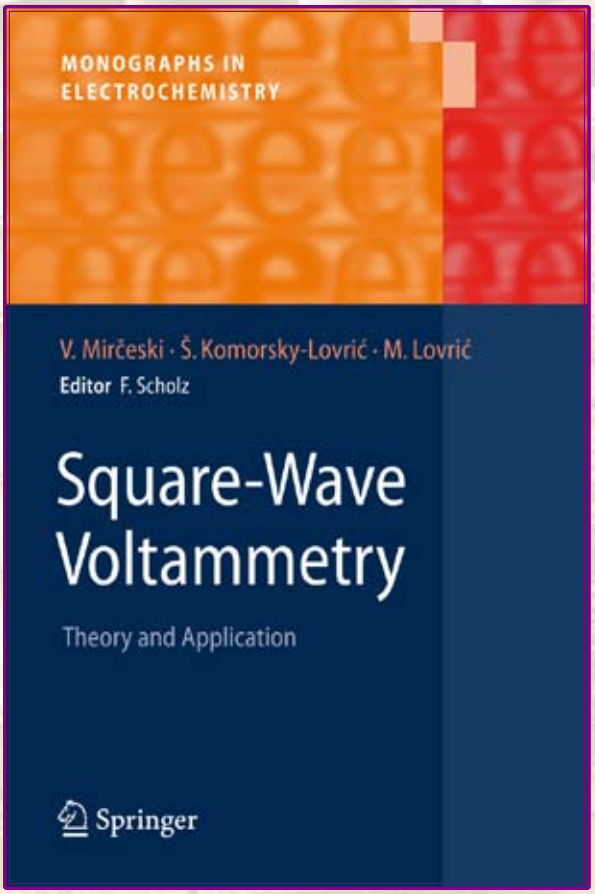


Figure 4. Front page of Square-Wave Voltametry by Mirčeski, Komorsky-Lovrić and Lovrić, 2007.

SELECTED PUBLICATIONS

Books

1. Komorsky-Lovrić Š, Lovrić M. Voltammetry. RBI, 2007 (in Croatian).
2. Legović T, van der Wel K, van Breusegen W. Guidelines for strategic environmental assessment. Ministry for Environmental Protection Physical Planning and Construction, Zagreb, 2007.
3. Mirceski V, Komorsky-Lovrić S, Lovrić M. Square-Wave Voltammetry, Springer, 2007.

Scientific papers

1. Bura-Nakić E, Krznarić D, Jurašin D, Helz, G. R, Ciglenečki, I. Voltammetric characterization of metal sulfide particles and nanoparticles in model solutions and natural waters. Anal Chim Acta 2007: 594: 44.
2. Ćosović B, Orlović Leko P, Kozarac Z. Rainwater dissolved organic carbon: Characterization of surface active substances by electrochemical method, Electroanalysis 2007: 19: 2077.
3. Dolenec T, Lojen, S, Kniewald G, Dolenec M, Rogan N. Nitrogen stable isotope composition as a tracer of fish farming in invertebrates Aplysina aerophoba, Balanus perforatus and Anemonia sulcata in central Adriatic, Aquaculture 2007: 262: 237
4. Dragun Z, Raspor B, Podrug M. The influence of the season and the biotic factors on the cytosolic metal concentrations in the gills of the European chub (Leuciscus cephalus L.). Chemosphere 2007: 69: 911
5. Frančišković-Bilinski S, Bilinski H, Grbac R, Žunić J, Nečemer M, Hanžel D. Multidisciplinary work on barium contamination of the karstic upper Kupa River drainage basin (Croatia and Slovenia); calling for watershed management. Environmental Geochemistry and Health 2007: 29: 69.
6. Filipović Marijić V, Raspor B. Metallothionein in intestine of red mullet, Mullus barbatus as a biomarker of copper exposure in the coastal marine areas. Mar Poll Bull 2007: 54: 935.
7. Gašparović B, Plavšić M, Bošković N, Ćosović B, Reigstad M. Organic matter characterization in Barents Sea and eastern Arctic Ocean during summer. Mar Chem 2007: 105: 151.
8. Grung M, Lichtenthaler R, Ahel M, Tollefsen

K-E, Langford, K, Thomas K V. Effects-directed analyses of organic toxicants in wastewater effluent from Zagreb, Croatia. Chemosphere 2007: 67: 108.
9. Jusup M, Geček S, Legović T. Impact of aquacultures on the marine ecosystem: modelling benthic carbon loading over variable depth. Ecological Modelling 2007: 200: 459.
10. Klanjšček J, Legović T. Is anchovy (*Engraulis encrasicolus*, L.) overfished in the Adriatic Sea? Ecological Modelling 2007: 201: 312.
11. Klanjšček T, Roger M, Nisbet R M, Caswell H, Neubert M G. A model for energetics and bioaccumulation in marine mammals with applications to the right whale. Ecological Applications 2007: 17: 2233.
12. Kuzmić M, Janeković I, Book J W, Martin P J, Doyle JD. Modeling the northern Adriatic double-gyre response to intense bora wind: A revisit. J. Geophys Res 2007: 111: C03S13.
13. Kwokal Ž, Komorsky-Lovrić Š, Lovrić M. Pollution of electrochemical laboratory by gaseous mercury. Fresenious Environmental Bulletin 2007: 16: 1238.
14. Lovrić M, Komorsky-Lovrić Š, Kahlert H, Scholz F. A model of mass transport near the tube wall in a flow-injection manifold, Anal Chim Acta 2007: 602: 75.
15. Žaja R, Klobučar RS, Smital T. Detection and functional characterization of Pgp1 (ABCB1) and MRP3 (ABCC3) efflux transporters in the PLHC-1 fish hepatoma cell line. Aquatic Toxicol 2007: 81: 365.

Chapters in books

1. Komorsky-Lovrić Š, Lovrić M. Theory and application of square-wave voltammetry, *In* New research on electrochemistry, Elizabeth P. Vargus (ed.), Hauppauge, New York, USA : Nova Science Publishers, 2007. pp 1-44.
2. Svetličić V, Žutić V, Mišić T. Atomic force microscopy. *In* Methods in Molecular Biology, Abramović Ristov A. (ed.) RBI, Zagreb, 2007.

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 processes in the marine ecosystem, Danilo Degobbis
- Laboratory for ecology and systematic, Ana Travizu
- Laboratory for marine molecular toxicology, Renato Batel

OVERVIEW OF THE DIVISION

The mission of the Center for marine research is to study processes in the marine environment from the subcellular to the regional scale, especially in benthic communities and water columns. Besides basic research, the Center is involved in the monitoring of the Adriatic Sea for government purposes and leads several international projects (Interreg) concerning protection of the marine environment.

TOP ACHIEVEMENTS

Long-term changes in the northern Adriatic ecosystem

A decrease of phosphorous availability in the Northern Adriatic ecosystem was mainly related to a reduction of the Po River discharge, being extremely low, particularly in spring, in almost all years since 2003. Lower availability of phosphorus can trigger a series of events in the ecosystem resulting in mucilaginous aggregate formation in favourable years. Over the last decade increased frequency of such events was noted.

Microbial heterotrophic activity along the gradients

The analysis of long-term variations in the abundances of bacteria and nanoflagellates along the eutrophication gradient Rovinj – Po Delta showed its significant impact on the dynamics of analyzed population, most pronounced in heterotrophic bacteria. The importance of the “top-down” control of heterotrophic bacteria by heterotrophic nanoflagellates’ predation declines spatially (from the eastern to the western part of the Rovinj – Po Delta profile) and temporally (from 1990 onwards), indicating changes in the ecosystem related to eutrophication.

Low impact of marine fish farming on sediment and meiofauna in the Limski Channel

A field study of the impact of fish-cage farming (sea bass, *Dicentrarchus labrax*, and sea bream, *Sparus aurata*) on sediment

and meiofauna was performed in the Limski Channel (northern Adriatic, Croatia). In the aquaculture area, sediment was characterized by markedly increased organic carbon, polyunsaturated fatty acid, and lipid concentrations with respect to the reference area. As a consequence, the total meiofauna abundance was lower in the fish-cage area, due to reduced contributions of copepods and other taxa, although the contribution of nematodes was higher than in the reference area.

These results suggest that a localized effect of fish farming waste occurred, with no serious oxygen disturbances, confined to the area directly underneath the cages. Although the sedimentological characteristics of the Limski Channel favour accumulation and have pronounced memory for highly degradable organic matter, the impact of the fish farming turned out to be negligible. These results suggest that sea bass and sea bream farming in the investigated system is eco-sustainable, not significantly altering the semi-enclosed marine ecosystem (Najdek et al., 2007).

First record of Ostreopsis cfr. ovata in the northern Adriatic Sea

Ostreopsis cfr. ovata is an epiphytic potentially toxic dinoflagellate species belonging to the genus Ostreopsis whose blooms have been related to human health problems, such as breathing and skin irritation. The first record of Ostreopsis cfr. ovata in the northern Adriatic Sea was reported from the Gulf of Trieste and the Rovinj coastal area, where the species was isolated from macro algae (Monti et al., 2007).

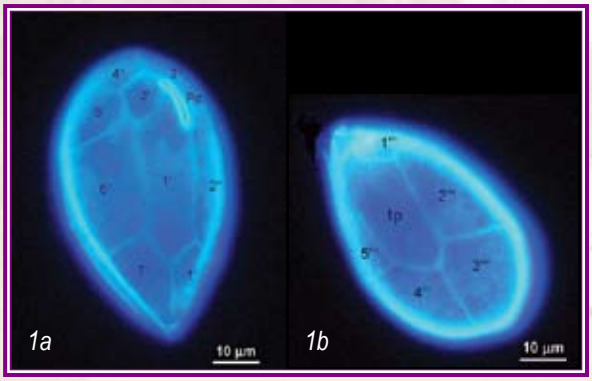


Figure 1a. LM epifluorescence. Epithecal view of O. cfr. ovata.
Figure 1b. LM epifluorescence. 'Hypothecal view of O. cfr. ovata.

Short term impact of planctonic mucilage aggregates on macrobenthos

A short term effect of planctonic mucilage aggregates on selected macrobenthic species (Arca noae, Cystoseira species and Verongia aerophoba) along the Istrian rocky coast was studied. The mucilage impact was species dependent. It was lethal for 5-45% specimens of the mollusc Arca noae, sublethal for the sponge Verongia aerophoba (partial necrosis for 7-56% of the colony surface) and apparently inoffensive for Cystoseira species, which were able to withstand the mucilage impact, since the necrosis was restricted to deciduous branches, while perennial parts of the thalli were not affected (Devescovi et al., 2007).

Deoxyribonuclease in the mussel *Mytilus galloprovincialis*

The presence of neutral DNase activity in bivalves was reported for the first time. The enzyme activity in four tissues of the mussel *Mytilus galloprovincialis* was analyzed by three different methods (i) specific denaturating SDS - PAGE zymogram, (ii) sensitive single radial enzyme diffusion (SRED) assay, and (iii) rapid and sensitive fluorimetric deter-

mination of DNase activity with PicoGreen. The fluorimetric assay was rapid and sensitive enough for determination of hydrolytic activity of dsDNA in mussel hepatopancreas, adductor, gills, and mantle. Maximal activity in all mussel tissue extracts was obtained in the presence of Ca^{2+} and Mg^{2+} at pH 7.0 with dsDNA as substrate. The neutral DNase activity in mussel tissue decreases in order hepatopancreas, mantle > gills > adductor. The enzyme activity displays inter-individual variability in particular tissue as well as variability among tissues within one specimen. In the hepatopancreas, one to three distinct proteins expressing neutral, Ca^{2+}, Mg^{2+}-dependent, DNase activity were detected by denaturating SDS-PAGE zymogram. This heterogeneity of neutral nucleases involved in DNA hydrolysis in hepatopancreas could reflect inter-individual variability in mussel food utilization and nutrient requirement (Bihari et al., 2007a; 2007b).

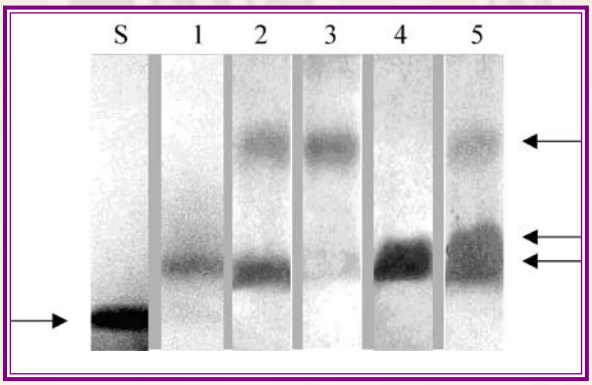


Figure 2. Heterogeneity of deoxyribonuclease isozymes in the mussel hepatopancreas.

Seawater toxicity along Adriatic coast – a long-term study

The objective of this study was the assessment of coastal seawater toxicity of 24 sampling sites along the Adriatic coast, Croatia, by the use of Microtox® bioassay. The database created in this study could serve to properly direct remedial activity and for the control of its efficiency. Analyses of temporal changes during a seven year period (1999-2005) showed a decrease of potential toxicity (EC_{50}) at 3 sampling sites and an increase at 2 sampling sites. Multivariate analyses (cluster, MDS) of the toxicity data set, using frequencies of different water quality as variables, were introduced. These analyses allowed discrimination of the sampling sites according to the distribution of toxicity with toxic load at each sampling site, related to the type of human activity in the area. This study also identified one hot spot, four potential hot spots and two sampling sites as unstressed control locations. Their spatial distribution revealed that the region of Split, Kaštela Bay is the area with the heaviest load of toxic agents (Fafanđel et al., 2007).

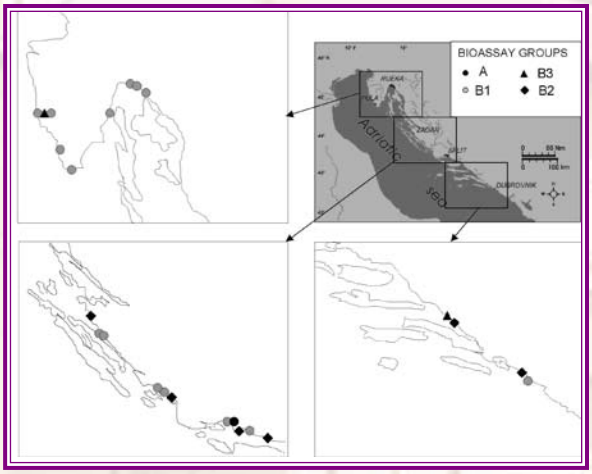


Figure 3. Spatial distribution of the toxicity data along Adriatic coast. A – fair water quality, B1 – medium water quality with higher frequency of fair water quality, B2 – medium water quality with lower frequency of fair water quality, B3 – low water quality.

Tracking of early biomineral growth in embryos

X-ray diffraction has been used to probe the growth processes of the first biominerals in early embryonal development. The latest data indicate that as soon as 12 hours after

fertilization, in the late multicellular embryonal development stage, well-formed crystalline material may be already detected, and that 24 hours after fertilization the first aragonitic prodissoconch I shell is formed. Significant quantities of a new crystalline phase were also detected and whose pending identification is expected to provide new insight into the crystal growth pathways and phase transitions in the biomineralization process.

Monitoring of larval development

Continued growth of embryos into the veliger larva stage has been monitored by following formation of the prodisoconch II shell over several days with scanning electron microscopy (SEM). The prodissoconch I/II boundary, marking the moment when the valves first completely enclose the larval body and close against one another, has been clearly determined (Fig.4, inset a).

Determination of the effects of environmental stress

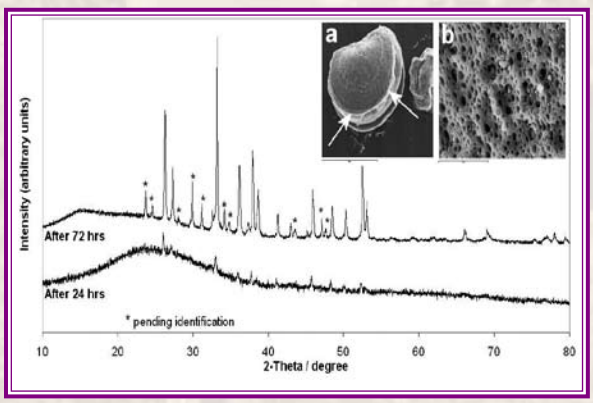


Figure 4. Powder diffraction data for Chione cancellata embryos. Inset - (a) SEM picture of the veliger larvae of Mytilus galloprovincialis (scale bar = 50 μm) and (b) SEM picture of valve internal surface morphology (scale bar = 30 μm).

The impact of changes in abiotic factors in the marine environment has been detected by the observation of uneven crystallization of the internal nacreous layer of the valve due to stress. This includes cases where elevated concentrations of nutrients (nitrates, nitrites, phosphates) in the northern Adriatic reduce the amount of dissolved oxygen (anoxia) during intensive phytoplankton blooms, causing both changes in the biomineralization process and morphological changes in the shell nacre (Fig.4, inset b).

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

1. Impact of pollution on programmed biosynthesis in marine invertebrates, Renato Batel
2. Ecotoxic effects of contamination on marine organisms, Nevenka Bihari
3. Biomineralization processes in marine organisms, Davorin Medaković
4. Structure and physiology of microbial communities in northern Adriatic fronts, Mirjana Najdek
5. Mechanism of long-term changes in the northern Adriatic ecosystem, Robert Precali
6. Biodiversity of benthic communities in the Adriatic: natural and human impacts, Ana Travizi

Programs supported by the Ministry of Science, Education and Sport and led by members of the Division

1. Natural and anthropogenic impacts on the Adriatic Sea ecosystem, Renato Batel
2. Croatian national monitoring programme Systematic research of the Adriatic Sea as a base for sustainable development of the Republic of Croatia (Project “Adriatic”), Nenad Smodlaka

Research, developmental and international projects

1. Schwaemme aus Rovinj (Kroatien)-Extractbereitstellung und Marikultur, Project: Molekulare Biotechnologie und Wirkstoffe mariner Schwaemme sowie Schwamm-assoziierter

Mikroorganismen, Renato Batel, Werner E.G. Müller (Croatian German scientific project)
2. Biocapital, Marie Curie Research Training Network, Renato Batel, Werner E.G. Müller (EU-FP6, 2005-2008)
3. Sponges, Renato Batel, Werner E.G. Müller (EU-FP6, 2005-2007)
4. Biosensor methods for the assessment of the effects of pollution, Renato Batel, Werner E.G. Müller (Croatian German scientific project)
5. 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, extension 2007-2008)
6. Integrated system for monitoring and forecasting of meteorological and water conditions parameters in the Adriatic Sea (ADRIAMET), Danilo Degobbis (EU INTERREG IIIA, 2004-2008)
7. Anossie attuali nel nord Adriatico, registrazione nei sedimenti in epoca storica, influenza sulle risorse di pesca e bentoniche. Modellizzazione e previsione (ANOCSIA), Robert Precali (Ministero dell'Istruzione, dell'Università e della Ricerca della Repubblica Italiana 2004-2008)
8. Monitoring of the marine coastal current of the North Adriatic (NASCUM), Nenad Smodlaka (2007-2008)

SELECTED ORGANIZED CONFERENCES

In Rovinj, from 08-12 October 2007, a scientific conference entitled Long Time-Series Observations in Coastal Ecosystems: Comparative Analyses of Phytoplankton Dynamics on Regional to Global Scales was held. It was organized by the American Geophysical Union, as a Chapman Conference, and the Center for Marine Research.

This Conference compared phytoplankton dynamics in coastal marine ecosystems where perturbations from terrestrial, atmospheric, oceanic sources and human activities converge to cause changes that ramify across local and global scales. The objective was to assemble and synthesize multi-decade observations toward quantitative and descriptive depictions of phytoplankton variability as an indicator of environmental change across the full diversity of coastal ecosystem types. The visions were a global phenology of phytoplankton at the land-sea margin and a conceptual model from which coastal ocean observing systems can be built. The Conference was attended by 80 scientists from 24 countries around the globe.

SELECTED INVITED LECTURES

1. Hamer B. The marine research station – Rovinj, School of Conservation Biology of the Croatian Biological Society -1885. Rovinj, Croatia, June 21-29, 2007.
2. Hamer B, Jaklin A, Batel R, Mueller WEG. Sustainable use of marine organisms - Project SPONGES, School of Conservation Biology of the Croatian Biological Society - 1885. Rovinj, Croatia, June 21-29, 2007.
3. Hamer B, Medaković D, Kanduč T, Mueller WEG, Batel R. Calcification on molluscs: Mussel *Mytilus galloprovincialis* as an indicator of marine environmental stress - A field study Project Adriatic", *German-Egyptian Year of Science and Technology* -Bioactive Natural Products: Current Status and Future Scenarios / Esmat Abdel Ghaffaar (ed.). Cairo, Egypt, September 16-17, 2007.
4. Smodlaka N, Đakovac T. Climate Changes and the Adriatic, Climate Changes – New Challenges through Regional Perspective, Jožef Štefan Institute, Ljubljana, Slovenija, December 4, 2007.

SELECTED PUBLICATIONS

1. Najdek M, Travizi A, Bogner D, Blažina M. Low impact of marine fish farming on sediment and meiofauna in Limski channel (northern Adriatic, Croatia). Fresenius Environ Bull 2007: 16: 784.
2. Monti M, Minocci M, Beran A, Iveša Lj. First record of Ostreopsis cfr. ovata on macroalgae in the Northern Adriatic Sea. Marine Poll Bull 2007: 54: 598.
3. Devescovi D, Iveša Lj. Short term impact of planctonic mucilage aggregates on macrobenthos along the Istraian rocky coast (Northern Adriatic, Croatia). Marine Poll Bull 2007: 54: 887.
4. Bihari N, Fafanđel M, Perić L. Tissue distribution of neutral deoxyribonuclease (DNase) activity in the mussel *Mytilus galloprovincialis.* Comp Biochem Physiol B 2007a: 147: 550.
5. Bihari N, Fafanđel M, Piškur V. Polycyclic aromatic hydrocarbons and ecotoxicological characterisation of seawater, sediment and mussel *Mytilus galloprovincialis* from the Gulf of Rijeka, the Adriatic Sea, Croatia. Arch Environ Contam Toxicol 2007b: 52: 379.
6. Fafanđel M, Bihari N. Temporal and spatial variations of seawater toxicity along Adriatic coast, Croatia: A long-term study. Fresenius Environ Bull 2007: 16: 1457.

Centre for Informatics and Computing

CIR

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

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, Nikola Pavković
- Information systems, Neven Kmetić
- Service and maintenance, Đuro Kuzumilović

OVERVIEW OF THE CENTRE

The mission of CIR is, through its scientific and research programme, to advance the usage of computers in scientific work. Specifically, we aim to do this by developing e-science technologies, as the next generation of knowledge infrastructure to support computationally based science. The realization of a national research project and program, as well as extensive international collaboration provides evidence for our advancement of the aforementioned mission. Specifically, in addition to ongoing collaborations with scientists in Switzerland, Slovenia, Hungary, and Bulgaria, CIR was involved in the sharing of contracted collaborative work based on an EU FP6 framework programme with 118 EU institutions. CIR is also a member of NESSI – the Networked European Software and Services Initiative caried out as part of the European Technology Platform on Software and Services. At the same time, CIR continues to remain active in the development and maintenance of the RBI's ICT infrastructure and provision of various services and support measures.

TOP ACHIVEMENTS

Project initiatives

Significant effort was expended in the Centre in 2007 towards the procurement of sustainable funding from external sources, with a particular focus upon the European Framework Programmes (FP). Following the successful involvement with four FP6 projects (see below), CIR prepared seven EU FP7 project proposals for ICT Calls. Four of these have successfully entered the negotiation phase. The project proposal COMANDS is on the reserve list for negotiation, while the other two project proposals are currently being evaluated. We plan to use the resources

obtained in this way to continue to expand the e-Science program and strive towards establishing a project chain along the lines of e-Infrastructure, distributed computing, parallel applications and scientific visualisation technologies.

FP6 Project successes

In the EU FP6 SEE-GRID-2 project, as the leader of the Work Package (WP) 4, CIR actively worked on the collection and systematisation of gained knowledge on Applications Gridification, acting as the editor of a Deliverable to the EC.

CIR, together with the Faculty of Graphical Arts, a university institution which is perceived as very important in the general direction of CIR towards Scientific Visualisation, is working on a Grid Application called VEPPAR (Visual Parallel Processing and Rendering). The first version of this Application was already used in educational activities.

In second quarter of year we started to realise an EU-FP6 project with the aim of establishing a Centre of Excellence for Scientific Visualisation. The CenVis is envisaged to be a prime point for the development of Scientific Visualisation, specifically in view of the modern developments towards 3D, stereoscopic presentation, in the Grid environment. Recently, we have been working on launching the project web-site and providing the work package tasks. The end of year saw the beginning of the adaptation investment to provide work space for Centre of Scientific Visualisation and a server point for hosting eInfrastructure and eScience support equipments.

eScience Development Activities

During 2007 CIR continued the eScience programme based on ICST (Information Communication Science Technology) on Grid platforms. This programme was initially based on the National Grid Initiative poly-project CRO-GRID, which was very successfully finished. Based on the experience of the CRO-GRID poly-project, during 2007 the CRO NGI (Croatian National Grid Infrastructure) was established, with important and constant contribution of CIR 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 particular, a new 96 processor HP blade cluster was installed as an extension to CRO-NGI.

The CRO-GRID JRU (Joint Research Unit), initiated during 2006, continued the work of the EU FP6 EGEE-II project throughout 2007. As part of the JRU, CIR continued as the leader of NA2 (dissemination) and NA4 (applications). Specific attention was given to the promotion of the NA4 activity of “Grid Service Library Applications” development, which focuses upon algorithmic systems applications.

Figure 1. New 96 processor blade cluster in CRO NGI

Introduction of the Quantum Random Bit Generator Service.

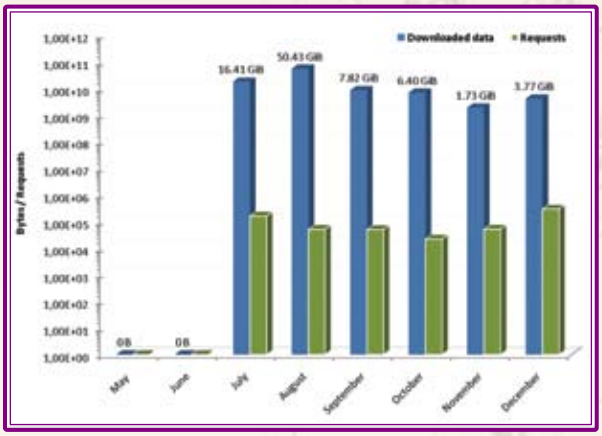


Figure 2. Monthly traffic at http://random.irb.hr in 2007.

The Quantum Random Bit Generator Service (QRBGS), is a network service intended for people that require truly random number sequences. It has been designed and developed trying to maximize data randomness, speed, accessibility, and robustness. Transparent access to the service is available from several major programming environments (C, C++, Java, Python, Perl, MATLAB), and for all major platforms (Windows, Linux and MacOS). Stand-alone clients and limited web access are also available.

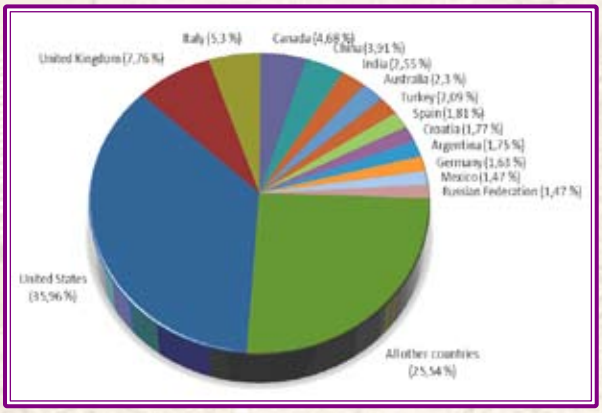


Figure 3. Countries of origin for users registered at http://random.irb.hr (5645 registered users in 2007).

Although the QRBGS was conceived primarily for stochastic simulations and scientific applications, it went public during July 2007, soon establishing itself as a free and unlimited general-purpose resource of high-quality random numbers online (http://random.irb.hr).

Monthly activity is depicted in Figure 2, showing that the amount of downloaded random data per month varies from 1.7 GiB to over 50 GiB, and the number of requests per month varies from 20 thousand to around 160 thousand. A breakdown of registered users by countries is given in Figure 3, showing that majority of users come from the United States. The majority of most active users originate from academia and research institutions. During the last half of 2007, 5645 registered users downloaded 86.56 GiB of random data. Throughout the same period, the web page of the service had 2.5 million hits, 150 thousand visits, and web upload traffic of 20.1 GiB.

The Virtue system

During 2007, the Virtue system was presented to the scientific community. Virtue is a new computer language and its auto parallelising implementation is specifically geared towards effective execution of complex algorithms written in a relatively simple way on distributed computing resources. Virtue is part of an effort towards the Grid Service Library Applications approach, as its main Grid purpose is to serve as a simple, yet powerful mathematical processing service, http://grgur.irb.hr/Virtue.

Information Systems development and service usage

The Information Systems Department continued their efforts to integrate the AAI@EDU.HR LDAP database with ActiveDirectory database from the Institute's headquarters, aiming to create a unified *Single Sign On* infrastructure that ensures the basic Services at RBI.

Services usage statistics

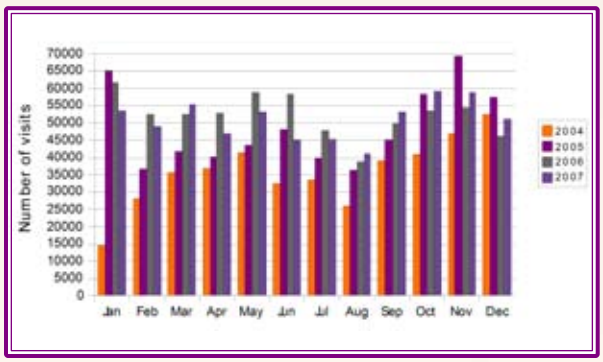


Figure 4. Web server statistics [www.irb.hr].

The main web-server (www.irb.hr), which provides information to the general public, is also maintained by CIR. The CMS-driven core engine enables users to develop extended functionality web applications such as time-schedule applications etc. In 2007, the web server statistics showed a minimal decrease in number of visits, comparing to the previous year.

GRID enabled clusters egee.irb.hr and grid1.irb.hr

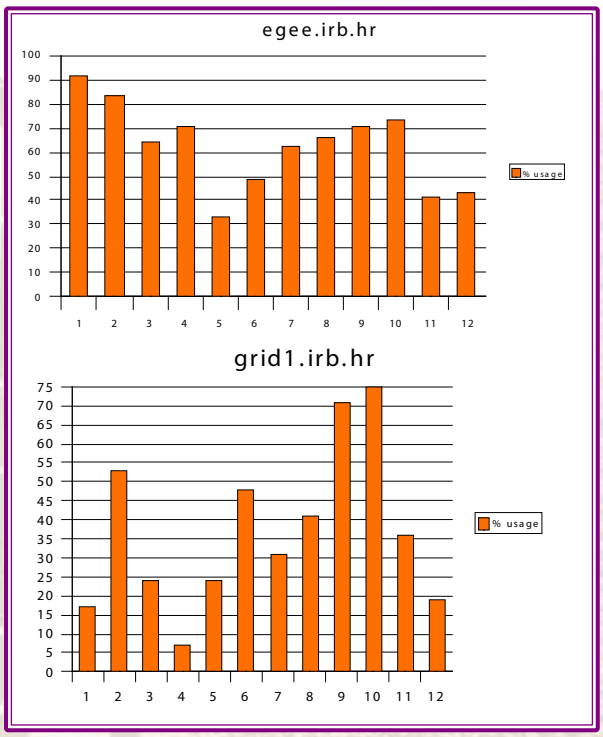


Figure 5. Web server statistics [www.irb.hr].

Both egee.irb.hr and grid1.irb.hr are GRID-enabled clusters, situated at the RBI. They are connected to the pan-european GRID project EGEE. As such, both clusters provide computational power to local but also foreign users coming from universities across Europe. The usage statistics shows reasonable load distributed among all months of the year.

Hardware/network infrastructure

A number of active network devices were acquired with aim of extending the existing network capacity of the RBI core network. These include Cisco network-switches and a Cisco Supervisor module for the core router.

Service and maintenance department

Our helpdesk is continuing its usage of OTRS Ticketing System, which has proven itself to be an indispensable tool for our everyday operations. Printing and TCR services continue to function without any interruptions. The IRB webpage is showing a steady increase in unique visitors. The web site is being monitored by our own local open-source AWStats system and Google Analytics. Overall it's business as usual in Services and Maintenance department.

Software products

In 2007, two new software products were developed. These were: Virtue v0.2 (mentioned above) and BarcaBase – A web application that allows entry of data on exons, and on individual analyses (including their melting profiles).

EDUCATIONAL ACTIVITIES

CIR provides 5 undergraduate and 3 graduate courses at the Faculty of Electri-

cal Engineering and Computing and the Faculty of Graphical Arts at the University of Zagreb. In addition to these activities, 2007 saw the organization of several specialized educational events. These were: GI – Grid Infrastructure (http://www.irb.hr/hr/cir/education/courses/gi), GA – Grid Applications (http://www.irb.hr/hr/cir/education/courses/ga), GD – Development and Porting Applications on the Grid (http://www.irb.hr/hr/cir/education/courses/gd), GBlast – Bioinformatics – Deploying BLAST on the Grid (http://www.irb.hr/hr/cir/education/courses/gblast), and P^3G^2 – Parallel Programming in Cluster and Grid Environment (inside the frame of MIPRO Opatija, http://www.irb.hr/en/cir/education/courses/gd).

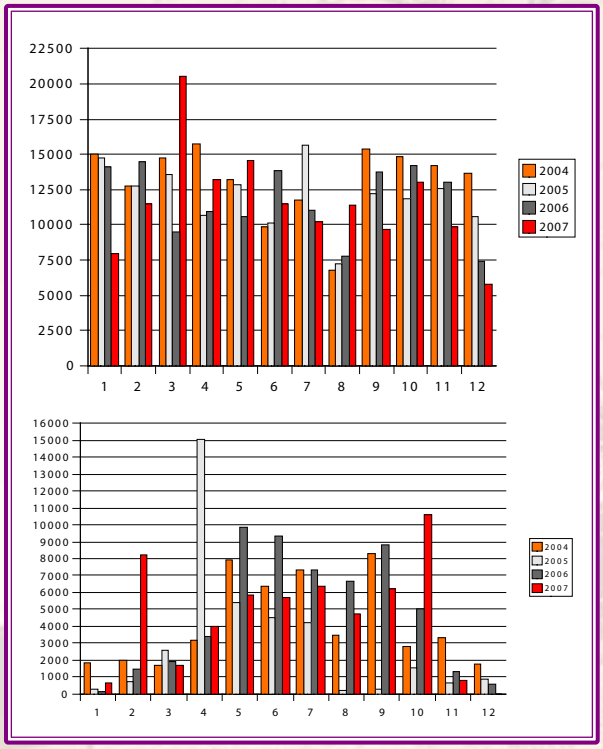


Figure 6. Total number of A4 printouts (2004-2007), and the number of printed posters (in cm 2004-2007.

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). Under the sponsorships of European Universities Sport association, CIR supported the first European Universities Sailing Cup with advance GPS tracking technology based on the Google Earth interface (www.sailing.hr).

PROJECTS AND PROGRAMS

Projects supported by Ministry of Science, Education and Sport

1. Scientific Visualisation Methods, Karolj Skala

Figure 7. CIR eScience workshop 18.12.2007.

Programs supported by the Ministry of Science, Education and Sports and led by members of the Division

1. Scientific program: Distributed Computing and Visualisation (2007-2012), Karolj Skala

International EU FP6 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 eInfrastructure Development 2 (SEE GRID 2) EU FP6, Con. No. 031775, Karolj Skala
4. Centre for Scientific Visualisation (CenVis), EU FP6, Con. No. 043947, Karolj Skala

SELECTED PUBLICATIONS

1. Kolari D, Skala K, Dubravi A. Integrated system for forest fire early detection and management. Period Biol 2007: 110: 6.
2. Stevanović R, Topić G, Skala K, Stipčević M, Medved Rogina B. Quantum random bit generator service for Monte Carlo and other stochastic simulations. Lecture notes in computer science. Berlin: Springer-Verlag, 2008. pp. 287-292.

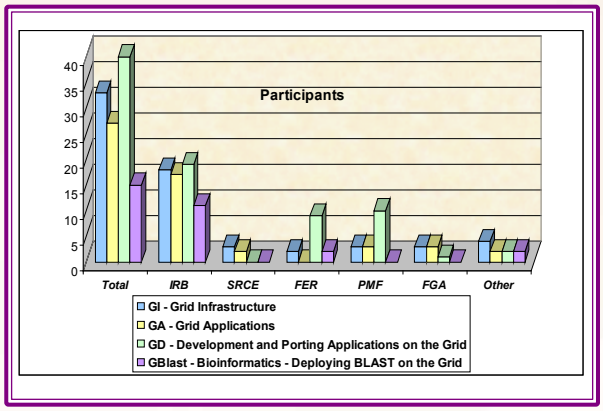


Figure 8. ***Statistical data on the educational activities GI, GA, GD and GBlast.***

Centre for Nuclear Magnetic Resonance

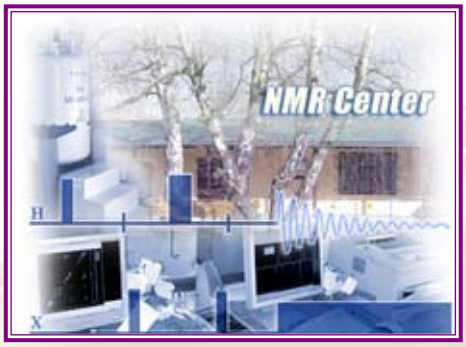
http://www.irb.hr/en/nmr

ORGANIZATION OF THE CENTRE

Head: Dejan Plavšić (replacement for Dražen Vikić-Topić)

The Center for NMR consists of the following groups:

- NMR group,
  Dejan Plavšić (replacement for Dražen Vikić-Topić)
- Glass group,
  Andrea Moguš-Milanković
- Immunochemistry group
  Nikola Štambuk



OVERVIEW OF THE CENTER

The Center for Nuclear Magnetic Resonance (NMR), the only academic NMR facility in Croatia, was established in November 2003 as an independent unit of the Ruđer Bošković Institute. The Center 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 Center also provides educational and professional support for researchers from governmental institutions and pharmaceutical industry.

Research work at the NMR Center 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 support the experimental measurements. Part of the investigation is focused on natural compounds and photochemistry products. The Center is also involved in the research of microscopic and macroscopic properties of various materials such as glasses, glass-ceramics and ceramics. Various types of nano- and micro-structured materials have been investigated using different techniques, including Impedance Spectroscopy (IS) and Thermally Stimulated Current (TSC). Another activity of the Center includes the testing of statistical methods and algorithms for the modelling procedures, research on viral immune response, defining relevant alpha-melanotropin and Prostate specific antigen (PSA) epitopes with related complementary peptides-paratopes.

The scientists from the Center participate in teaching at the undergraduate and graduate studies at Universities of Zagreb, Rijeka, Osijek and Dubrovnik. Active collaborations are maintained with research groups from the USA, Turkey, Austria, Slovenia, Macedonia, Brazil, Russia, and the Czech Republic. The research also includes the application

of the following equipment at RBI: Bruker Avance 300 and 600 MHz NMR spectrometers. The subsidiary of NMR Center, located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb, uses Varian Gemini 300 MHz NMR spectrometer.

Figure 1. The instrumental room with a 14T magnet (600 MHz frequency for ^{1}H NMR).

well as ^{1}H-^{1}H spin connectivity maps from the two-dimensional frequency domain heteronuclear long-range correlation data matrix (Schoefberger et al., 2007).

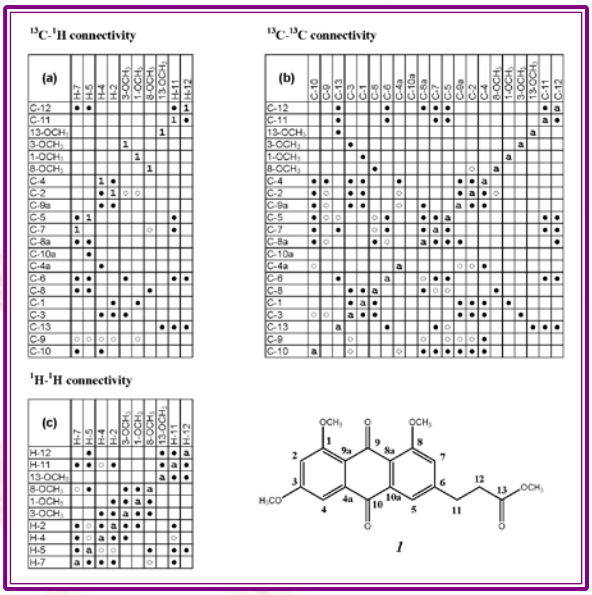


Figure 2. For convenience and data storage economy, the correlation spectra can be compressed into connectivity maps like these of compound ***1****: (a) ^{13}C-^{1}H connectivity, (b) ^{13}C-^{13}C connectivity, (c) ^{1}H-^{1}H connectivity, 1 - one bond H-C correlation, a - auto-correlation, ● - strong correlation, ○ - weak correlation.*

TOP ACHIEVEMENTS

Covariance processing of HMBC experiments to obtain homonuclear long-range correlation spectra

A new application of covariance nuclear magnetic resonance processing was presented based on ^{1}H,^{13}C-HMBC experiments which provides an effective way for establishing indirect ^{1}H-^{1}H and ^{13}C-^{13}C nuclear spin connectivity at natural isotope abundance. The method, which identifies correlated spin networks in terms of covariance between one-dimensional traces from a single decoupled HMBC experiment, derives ^{13}C-^{13}C as

Synthesis and structural characterization of polymeric mercury(II) complexes

Novel mercury(II) compounds of 3-hydroxypicolinic acid (HpicOH) were synthesized and characterized. HgCl(picOH) and $HgBr_2$(HpicOH) were obtained as reaction products from the reaction of the corresponding mercury(II) halide with HpicOH, irrespective of the molar ratio of the reactants. From the reaction of HpicOH and mercury(II) acetate, $Hg(picOH)_2$ was obtained. ^{1}H and ^{13}C NMR spectroscopic data were analyzed for all three complexes (Popović et al., 2007).

Melting temperature effects on the structure of phosphate glasses

The physical and chemical properties of phosphate glasses can be optimized by controlling the melting conditions and chemical composition. The effects of melting temperature on the structure and iron redox equilibrium of zinc iron phosphate glasses have been reported. The average iron valence and the configuration of the phosphate network were modified by varying the melt temperatures and investigated using Mössbauer, Raman and impedance spectroscopies.

The $Fe^{2+}/(Fe^{2+} + Fe^{3+})$ ratio increased from 0.18 to 0.38 as the melting temperature increased from 1100 to 1300°C. The measured isomer shifts showed that both Fe^{2+} and Fe^{3+} ions are in octahedral coordination. It was shown that the dc conductivity strongly depended on $Fe^{2+}/(Fe^{2+}+Fe^{3+})$ ratio in glasses. The dc conductivity increases with the increasing Fe^{2+} ion content in these glasses. The conductivity arises from the increase of polaron hopping from Fe^{2+} and Fe^{3+} ions (Reis et al., 2007).

Monte Carlo approach to the Estrada index

The Estrada index is a recently introduced molecular-structure descriptor. Using a Monte Carlo approach and treating the (molecular) graph eigenvalues as random variables, an approximate expression of very high accuracy was deduced for the Estrada index in terms of the number of vertices and number of edges (Gutman et al., 2007).

EDUCATION

Scientists from the Division contributed to 9 undergraduate and postgraduate courses in 2007 as part of the involvement in the educational programs of Universities in Zagreb, Osijek, Rijeka and Dubrovnik.

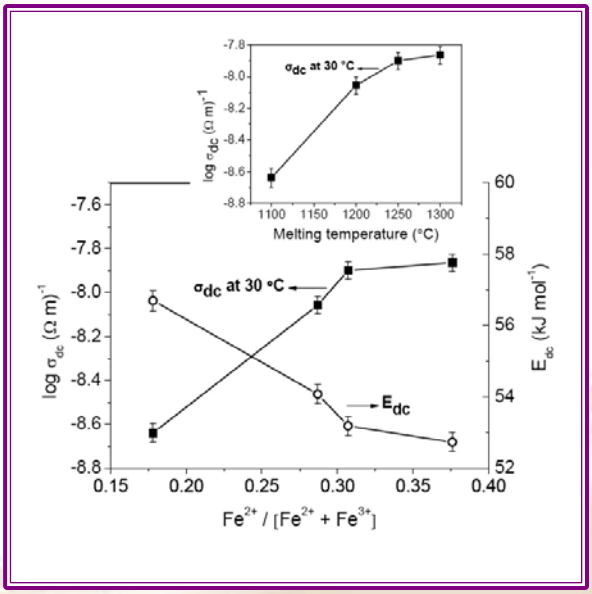


Figure 3. The dependence of the dc conductivity, σ_{dc}, at 30ºC and activation energy for dc conductivity, E_{dc}, upon the $Fe^{2+}/[Fe^{2+}+Fe^{3+}]$ ratio in the zinc iron phosphate glasses. Inset: dc conductivity, σ_{dc}, at 30ºC as a function of melting temperature. Lines are drawn connecting data symbols of each kind.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. NMR Spectroscopy and Modelling of Bioactive Molecules, Dejan Plavšić
2. Influence of structure on electrical properties of (bioactive) glasses and ceramic, Andrea Moguš-Milanković
3. Modelling of bioactive molecules and testing of their properties and activity, Nikola Štambuk

Research, developmental and international projects

1. NMR Methods for Structural Analysis of Peptidoconjugates, Vilko Smrečki (Dražen Vikić-Topić), (MSES, bilateral collaboration with Austria, WTZ 16/06)
2. NMR Study and Modelling of Pharmacologically Applicable Peptides, Željko Marinić (Dražen Vikić-Topić), (MSES, bilateral collab-

oration with Slovenia, 910-08/05-01/00165)
3. The origin of structural defects and their influence on macroscopic properties of solar silica glass, Davor Gracin (Andrea Moguš-Milanković), (NZZ, Ruđer Bošković Institute-Lipik Glas, doo)

Contracts with industry

1. Collaboration Contract with PLIVA d. d. Pharmaceutical Industry
2. Collaboration Contract with BELUPO d. d. Pharmaceutical Industry
3. Collaboration Contract with the Croatian Institute of Viticulture and Enology
4. Collaboration with Lipik glas doo, Glass Industry

SELECTED INVITED LECTURES

1. Smrečki V, CSA Tensor Calculation of Peptide Backbone Atoms: Dependence on Conformation and Hydrogen Bonding, Mayo Clinic and Foundation, NMR Facility, Rochester, MN, USA, March 06, 2007.
2. Šantić A. Structure and electrical properties of phosphate glasses, Croatian Microscopic Society, March 07, 2007.
3. Konjevoda P, Štambuk N, Pokrić B. Statistical analysis of DNA microarray data: Limitations and perspectives in The 22nd International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik, Croatia, June 11-16, 2007.
4. Štambuk N, Konjevoda P, Vikić-Topić D, Pokrić B. Modelling of Epitope-Paratope Interaction Using Molecular Recognition Theory in The 22nd International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik, Croatia, June 11-16, 2007.

SELECTED ORGANIZED CONFERENCES AND COURSES

1. The 22nd Dubrovnik International Course & Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Dubrovnik, Croatia, June 11-16, 2007, organized jointly by D Plavšić, D Vikić-Topić, N Štambuk, P Konjevoda (NMR) and A Graovac (ZFK).
2. 4th International Summer School and European School on Solid State NMR: Solid State NMR for Liquid State NMR Spectroscopists, Dubrovnik, Croatia, September 16-21, 2007, organized by V Smrečki and D Vikić-Topić.

SELECTED PUBLICATIONS

1. Gutman I, Radenković S, Graovac A, Plavšić D. Monte Carlo approach to Estrada index. Chem Phys Lett 2007: 446: 233.
2. Popović Z, Matković-Čalogović D, Popović J, Vicković I, Vinković M, Vikić-Topić D. Coordination modes of 3-hydroxypicolinic acid: Synthesis and structural characterization of polymeric mercury(II) complexes. Polyhedron 2007: 26: 1045.
3. Schoefberger W, Smrečki V, Vikić-Topić D, Müller N. Homonuclear long-range correlation spectra from HMBC experiments by covariance processing. Magn Reson Chem 2007: 45: 583.
4. Škorić I, Marinić Ž, Molčanov K, Kojić-Prodić B, Šindler-Kulyk M. Complete ^{1}H and ^{13}C NMR assignment of *trans*,*trans*-2,3-divinylfuran derivatives. Magn Reson Chem 2007: 45: 680.
5. Reis ST, Moguš-Milanković A, Ličina V, Yang J, Karabulut M, Day DE, Brow RK. Iron redox equilibrium, structure and properties of zinc iron phosphate glasses. J Non-Cryst Solids 2007: 353: 151.
6. Šantić A, Moguš-Milanković A, Furić K, Bermanec V, Kim CW, Day DE. Structural properties of Cr_2O_3-Fe_2O_3-P_2O_5 glasses, Part I. J Non-Cryst Solids 2007: 353: 1070.

Library

http://library.irb.hr

Head of Library: Jadranka Stojanovski

OVERVIEW OF LIBRARY ACTIVITIES

Research institutes, such as the Ruđer Bošković Institute, function in a world of ideas, concepts, and knowledge. The new knowledge that emerges from institutions such as RBI has traditionally been reviewed, organized, and shared across the scientific community in the form of journals, books, dissertations, reports, conference papers etc. It is the mission of the RBI Library to acquire, organize, and maintain this information, in whatever form they may take, for the benefit of current and future generations of scholars

.

The RBI is both a consumer and a producer of information. The Institute relies heavily on the availability of such organized information as a backbone of successful research. The RBI also contributes significantly to the stream of publications that flows inside the scientific community. With enhanced support, the Library is preparing to take on activities that capture and preserve the intellectual contributions of RBI employees. Also we plan to collaborate with our colleagues more closely to select and manage different forms of information that will contribute daily to the RBI's excellence in research and teaching.

GOALS AND OBJECTIVES

The Library's mission is to provide access to resources, instruction, and services that are most important to the RBI's objective of advancing scholarship in the fields of natural sciences and biomedicine. The Library is committed to offering services that promote research and meet their information needs. In pursuit of this mission, the Library provides information and materials through a wide range of print and electronic resources.

The main objectives are focused on the development of a strategic plan for the implementation of an institutional repository, 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.

MEMBERSHIPS

The RBI Library is an active member of EURASLIC (European Association of Aquatic Sciences Libraries and Information Centres). This year, a member of the Library staff participated in the biennial EURASLIC conference, which was held in Karadag (Krimea, Ukraine) under the working title "From Treasures of the Seas - to Treasures of the Libraries". A fruitful international collaboration with library-members of EURASLIC is continuing. Within EURASLIC, the RBI Library participates in several activities and projects:

- ODINECET (Ocean Data and Information Network for European Countries in Economic Transition)

- MedSIG - Mediterranean Special Interest Group (network of aquatic libraries and information centres in the Mediterranean region)

- IAMSLIC Z39.50 Distributed Library (joint online catalogue of International Association of Aquatic and Marine Science Libraries and Information Centres)

- Extensive international interlibrary loan network.

Figure 1. EURASLIC conference participants.

As a part of its involvement in EURASLIC activities, the RBI Library participated in a training course within the framework of the ODINECET project. The Training was sponsored and hosted by the UNESCO/IOC Project Office for IODE in Oostende, Belgium, from November 19-23, 2007. The Course was attended by 13 participants from 7 countries (Bulgaria, Croatia, Estonia, Latvia, Poland, Russia and Ukraine). The main topics were devoted to the theoretical and practical steps involved in the creation of an electronic document repository. Other advanced topics on marine information/data partnering, current integrated library systems, and historical ecology/data mining and graphics were also presented. The RBI Library has already participated in the first level of this course organized in 2006.

COLLECTIONS

Digital collection

In 2007, the journal acquisition model continued to be realized through "big deals" with the world's main publishers, such as Elsevier, Springer, Wiley, Blackwell etc. This involves subscription on the national consortia level, directly by the Ministry of Science, Education and Sports. Besides the 20.000 e-journals available for the Croatian academic community, we experienced a 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 the newly developed Library portal to e-journals Pero (http://knjiznica.irb.hr/pero), which is heavily used across the Croatian academic community. RBI researchers can access over 60 bibliographic and full text databases, and over 20.000 peer-reviewed e-journals and 42 e-books online.

Printed collection

While the electronic resources account for most of our time and attention, print publications, even with their reduced numbers, still remain an important part of our collection and will continue to do so well into the future. In 2007, we subscribed only 72 printed journals (in addition to the electronic version). The book collection amounts to 21.682 volumes, 461 of which were newly acquired in 2007.

Interlibrary loan

The RBI Library collection, besides being a tool that facilitates research and scholarship at the RBI, serves a larger purpose. Library collections represent accumulated knowledge, which is important for research at the RBI, but also serve a global scholarly community. The RBI Library has a well-established interlibrary loan service with Croatian and foreign libraries. In 2007 it fulfilled 762 requests for documents made by RBI staff, and over 270 requests from other libraries. Interlibrary loan requests have been handled through an online application that was developed in-house. Through cooperation with numerous libraries we can offer an extensive shared collection of greater depth than any of the libraries could manage alone.

SERVICES

The RBI Library web-site is the place where we present and incorporate our digital collections and services. It is also the main access point to the online catalogue and networked resources. In 2007, 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 the 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 allowing much of the basic 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)
- Centre for online databases (http://www.online-baze.hr)
- Portal for Croatian scientific journals - HRČAK.

NEW LIBRARY MANAGEMENT SYSTEM

In 2007, the new Library Management System, which was evaluated and selected by Croatian National and University Library for all Croatian higher education and research libraries, was still not implemented. The Voyager system was chosen to support library functions such as acquisition, cataloguing, and interlibrary loans. Implementation of Voyager, which was expected early in 2007, would have permitted the RBI Library to utilize state-of-the art technology for delivering services. At the end of 2007, it was decided to undertake the migration to the integrated library system KOHA, which is an open source software available to every library and supporting all modules. As part of this migration, we converted the data to be compatible with the new software and performed the conversion of standards from UNIMARC to MARC21.

EDUCATION

During 2007 the Library staff members were involved in teaching graduate courses at University J. J. Strossmayer in Osijek. Regular trainings for scientists were held at University of Zagreb and other Croatian universities on database retrieval and optimal use of bibliographic and full text databases. In addition, in the process of helping library users formulate research strategies, identify information sources, and discuss methods of accessing resources, librarians educated those they assist (KEKS training).

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 StojanovskiCentre for online databases, Jadranka Stojanovski.

SELECTED ORGANIZED CONFERENCES

1. The Croatian academic and special libraries conference "Dial U for user: Libraries and their users", held at the Faculty of Electrical Engineering and Computing, University of Zagreb, Zagreb, from March 2-3, 2007, and organized by the RBI Library, Croatian Academic and Research Network CARNet and Faculty of Philosophy, University of Zagreb.

SELECTED LECTURES

1. Stojanovski J. Should the system of scientific publishing be changed? (in Croatian) CUC2007, 9th CARNet User's Conference, Rijeka, November 19-21, 2007.
2. Stojanovski J. Researchers, reachers and students as interactive creators of a new generation of digital libraries and librarian's role. LIDA 2007: Libraries in the digital age

Figure 2. Librarian's 2007 conference with user services as a main topic.

Figure 3. Conference at the glance.

held in Dubrovnik and Mljet, Croatia, May 28-June 02, 2007.

SELECTED PUBLICATIONS

Articles

1. Konjević S. E-journals today (in Croatian). Automatika 2007: 48: 183.
2. Macan B. Scopus – new generation data base (in Croatian). Kemija u industriji 2007: 52: 64.
3. Pikić A. Vodopijevec A. PERO – Data base of available e-journals with full texts (in Croatian). Kemija u industriji 2007: 56: 354.

Books

1. Stojanovski J. Online data bases - handbook. CARNet, Zagreb 2007 (in Croatian).

Ruđer Innovations Ltd.

http://www.r-i.hr

COMPANY ORGANIZATION

Head of Management Board, CEO: Domagoj Oreb

Member of Management Board, CFO: Paško Anić-Antić

Member of Management Board: Božidar Etlinger

Business Development Manager: Davorka Moslavac Forjan

Business Development Manager: Davor Aničić

Project Analyst: Matea Novosel

OVERVIEW OF THE COMPANY

Ruđer Innovations Ltd. (R-I) is a company owned by the Ruđer Bošković Institute (RBI), specializing in the commercialization of innovations and transfer of technology. The company links science and technology with economy and industry. We are open to the scientific community, including researchers and innovators, whom we help to commercialize their innovations and scientific research results. We are also open to enterprises wishing to apply the know-how of the scientific community in their businesses.

The activities of R-I include: discovery and evaluation of intellectual property, protection of intellectual property rights, and assistance in selecting and implementing an appropriate commercialization model (licensing, establishing spin-off companies, joint ventures). The company provides consultancy services for technology transfer and business agreements, as well as financial support for innovations and projects. We aim to help Croatian innovators and scientists and to make their knowledge more competitive on world markets.

ACHEIVEMENTS IN 2007

Establishment of spin-off companies

During 2007, R-I established 3 spin-off companies. Ruđer-Medikol Cyclotron Ltd. was set up to produce and develop radioactive nuclei for medical purposes. Ruđer-Medikol Diagnostics Ltd. deals in genetic testing for hereditary breast cancer, by using a sophisticated method developed in RBI laboratories, to be followed by other molecular genetic testing in the future. Initium Futuri Ltd. was founded in August 2007 by four young innovators and R-I with the goal to offer ICT solutions based on the latest development platforms.

Portfolio

The R-I portfolio currently contains 40 innovations and scientific projects with commercial potential, primarily from the fields of chemistry, medicine, biology, physics and informatics. Several of these have already been implemented in business and industry, while others are awaiting commercialisation. Licensing of innovations and know-how from our portfolio is but one method of commercialization of intellectual property engaged in by R-I. The database of innovations, projects, and spin-off companies is always available on the R-I web page (www.r-i.hr).

Expansion

Ruđer Innovations began its existence in 2006 with a single employee, 1 project, 1 patent application, and 1 licence. By the end of 2007, it had expanded significantly to the point where now it has 6 employees, 35 projects, 17 patent applications, 4 licences, and 3 spin-off companies. It is planned to continue this expansion into 2008 through the establishment of additional spin-off companies, the addition of dozens of new innovations to the portfolio, and the intensification of the connection between Croatian science and industry. By doing so, the aim is to establish R-I as a regional leader in the area of commercialization of science and technology.

Notes

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