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Ruđer Bošković Institute
Annual Report 2005



Ruđer Bošković Institute

Annual Report 2005



Zagreb, 2006.

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Welcome to the Ruđer Bošković Institute Annual report 2005. The report presents selected information and examples of the main achievements that illustrate the activity of the RBI in its main areas of work. Rudjer Bošković Institute, as the largest Croatian research institution, occupies a special position in the society, being on one side the most promising place for scientific carriers of many young Croatians, and on the other side it is perceived as the guarantor for faster development of Croatian society based on knowledge. Hence, to fulfil these expectations the consensual mission of the Institute incorporates three main tasks:

- to sustain and further develop the high quality of basic research in domains of physics, chemistry, biology, biomedicine and marine and environmental research,
- to contribute to higher education at Croatian universities particularly at the postgraduate level, and
- to create intellectual property, commercialize knowledge and collaborate with domestic industry and contribute to further economic development of Croatia.

These tasks may seem difficult and too ambitious, but the ongoing changes in almost all segments of the society including systems of education, economy, legal system, science and the technology sector are all aimed to approach the EU standards in the near future.

The following pages of the report show the fruits of the honest efforts and devoted work of our scientists, and also to which extent the mission of the Institute was fulfilled in 2005. To them and all staff goes my sincere thanks, and further to the Croatian Ministry of Science, Education and Sport, as our main funding institution. We sincerely hope that in the future we will do even better.

Director of Ruđer Bošković Institute
Professor Mladen Žinić, PhD



Introduction

INTRODUCTION

The overall performance of the Rudjer Bošković Institute in 2005 continued at the high levels attained in 2004. This year also saw the initiation of some new activities, such as increased efforts toward collaboration with domestic industry and regional Universities as well as partial reorganisation. Despite these new efforts, the level of achievement in basic research in chemistry, physics, biology, oceanography and biomedicine remained unchanged. The best results, achievements and activities of each of the RBI Divisions and Centres are highlighted in the following pages of this report.

Of the many important results realized in 2005, a select few rate specific mention. For example, the AFM imaging of the giant gel formed in the Northern Adriatic was performed for the very first time (Division of Marine and Environmental Research). Three young researchers of the Theoretical Physics Division developed a new approach to the numerical calculation of problems in electrostatics; their “Robin Hood” method shows excellent properties, surpassing the currently used methods in terms of both speed and accuracy. New important results were achieved in molecular medicine where DNA analysis of patients revealed a total of 5 different as yet uncharacterized point mutations in the SAHH gene, which causes serious health problems with a possible lethal outcome (Division of Molecular Medicine). Also the first steps toward nano-science

were described by researchers of Division of Materials Physics who successfully prepared silicon nanostructures. New inorganic materials including solid solutions, zeolites, new hydrogen storage materials (Division of Materials Chemistry) and supramolecular gels as new controllable soft materials (Division of Organic Chemistry) were prepared. Photo-induced conversion of DNA non-binding to DNA-binding molecules was reported which provides new concept of photodynamic cancer therapy. The synthesis of a new superbases HMPN, being the most basic “proton sponge” synthesized so far was also achieved (Division of Organic Chemistry). In addition to their research activities, the Centre for Information and Computing Sciences and the Library provided most valuable contributions in the information and communication sectors, being of the highest importance for the functioning of the entire Institute.

The majority of the scientific results produced in 2005 were published in high ranking international Journals. These scientific achievements should be considered with pride, particularly in the context of the considerable time and effort that was devoted to the first and usually most difficult steps towards reorganizing the Institute and redefining its goals and tasks. New tasks were defined in order to fulfil the needs of the developing Croatian economy and higher education system and to contribute to general development of the society in order to comply with the standards necessary for

the EU membership. On January 31, the new Statute and several other new documents were put into power which brought important novelties in the organisational structure and functioning of the Institute and also implemented new, higher standards for (scientific) professional promotion. The changes were designed to increase the efficiency of administration and management, to increase the quality and productivity of scientific research, to stimulate international scientific collaboration (particularly participation of RBI scientists in the networks constituting the European Research Area), to increase the contribution of RBI scientists in higher education and last but not least to enhance commercialisation of knowledge, innovations and intensify the collaboration with domestic industry. The changes included restructuring of the large and inoperative Scientific Council consisting of close to 130 scientists to a more operative body of only 29 members. By the Statute, the establishment of the Agency for innovations, an RBI owned company for the commercialization of knowledge, was instigated. In accordance with the goal of further RBI internationalisation, the International Scientific Board (ISB) was established in 2005 consisting of 5 eminent scientists from each field (chemistry, physics, molecular biology, biomedicine and oceanology) constituting a Board of 25 members altogether. Four distinguished members of the Board visited the Institute already in 2005: the Nobel Prize winner and the founder of supramolecular chemistry Prof. Jean-Marie Lehn, Prof. Egon Matijević from Clarkson University, Potsdam, USA; Prof. Werner Müller-a from Institut für Physiologische Chemie, Johannes Gutenberg-Universität

Mainz and, Prof. Helmut Schwartz from the Institut für Chemie, Technische Universität, Berlin. During the visit of Prof. Lehn, the collaboration with the Embassy of France in Zagreb was initiated. In November the Memorandum on Collaboration between the RBI and the Embassy of France in Zagreb was signed by the ambassador, his Excellency Mr. Francois Saint-Paul. By this agreement, the most generous financial support provided by the Embassy shall be used to cover the short visits to RBI of up to 3 eminent French scientists per year. Undoubtedly, such visits will contribute to further improvement of RBI science and also strengthen the collaboration between RBI and French scientists in various fields.

In 2005, the Institute continued with organization of the "Open Days" aimed to fully inform public on RBI activities and achievements. From the 21st to the 23rd of May, more than 4200 visitors entered the Institute's facilities, attended lectures on scientific activities and witnessed interesting experiments and use of sophisticated scientific equipment. It is highly encouraging that the vast majority of the visitors were young people; this fact reveals the high level of interest for science amongst the younger generation and suggests a rather safe future for Croatian science.

In March, the Institute hosted a delegation from the Netherlands headed by her Excellency Ms Maria van der Hoeven, Minister of Education, Culture and Science. In May, the Institute was visited by the Minister of State for Science and Technology of Japan, his Excellency Yasufumi Tanahashi and later the same month by a high level delegation from the Ministry of Science of India, headed by Mr. Y. P. Kumar, Head of International

Cooperation and Mr. S.K. Varshney, a scientist from the International Division. On that occasion the bilateral India-Croatia agreement on scientific cooperation and financial support for collaborative research projects was announced. It is noteworthy and impressive that the first call for the bilateral projects was announced already in September of 2005. In addition to those outlined above, the Institute hosted many other distinguished foreign guests during 2005. These included Walter Truett Anderson, the president of the World Academy of Art and Sciences, San Francisco; Prof. Frank Gannon, executive director of EMBO and Mr. Iain W. Mattaj, FRS, director general of EMBL, Dr. Viktor Stefov, Head of Department of Science, Ministry of Education and Science of the Republic of Macedonia, the directors or high representatives of the INRIA, Austrian Research Promotion Agency, European Commission Joint Research Centre, IC2 Institute of the University of Texas at Austin, NIH and NSF. In general, strengthening of the international collaboration particularly by active participation in the collaborative projects of EU networks was defined as one of the Institute's primary goals. In this context the meeting of the COST D27 action on the Prebiotic Chemistry and Early Evolution held in May at RBI, with participating group from the Department of Physical Chemistry and the acceptance of new COST B35 Action "Lipid Peroxidation Associated Disorders" proposed by RBI's Division of Molecular Medicine as the only COST action coordinated by Croatia should be mentioned here as two very encouraging examples.

In 2005 the Institute also started with first steps of the preparation of the first ever international evaluation of scientific performance. In this regard the help of the col-

leagues and experts from the Max Planck Gesellschaft, Dr. Berthold Neizert, Head of the Division of International Relations and Dr. Stefan Echinger, Head of the Division of Strategic Planning, who shared their experience with us during their short visit to the Institute, was most valuable.

In 2005 the RBI was endowed with valuable new equipment. Through the combined support of the Ministry of Science Education and Sports and IAEA, the Department of Experimental Physics became the owner of new Tandetron Accelerator. The small opening ceremony was witnessed by the Deputy Director General of the IAEA, Dr. Werner Burkhardt.

A number of foreign scientists have visited the Institute during 2005 and delivered interesting lectures. Traditionally, the RBI has organized the Institute's Colloquia for many years and in 2005 more than 30 lectures were delivered including more than 20 delivered by foreign scientists or by Croatian scientists working abroad. The member of the RBI International Scientific Board (ISB), Jean-Marie Lehn gave a lecture on "Supramolecular Chemistry and Self-Organisation by Design and By Selection" in a fully crowded lecture hall. Also the lectures of three other distinguished members of the ISB, Egon Matijević, Helmut Schwarz and Miroslav Radman were extremely interesting and very well attended.

To strengthen the collaboration with regional Universities and increase its contribution in higher education in natural science and biomedicine, the RBI signed agreements of cooperation with Universities of Split, Dubrovnik and Zadar. Shortly after, the preparations for the organization of joint post-graduate studies in Molecular Biosciences in collaboration with the Universities of Osijek

and Dubrovnik, on the Biology of Tumours in collaboration with the Universities of Split and Dubrovnik and on Biophysics in collaboration with the University of Split were begun. Also, a Letter of Intent concerning collaboration in scientific research, education and partnership in commercialization of knowledge was signed with the University of Zagreb. The activities of RBI in the sector of education were also extended to encompass collaboration with the High School of Business and Administration located in Zaprešić near Zagreb, where the biannual studies of project management in science and commercialization of knowledge were organized with the participation of the RBI experts. In September and December, two general contracts concerning collaboration in applied research with two major Croatian companies, namely Podravka Food Industries, Koprivnica and PLIVA Pharmaceutical Company, Zagreb, were signed and the first projects started. And last but not least, the first RBI spin-off company BioZyne was launched in 2005 in

collaboration with Alpe Adria Venture Fund, Vienna. The Company was established with the task to further develop the potential of compounds with anticancer activity discovered at the RBI. For the first time the RBI participated in ARCA – The International Exhibition of Innovations, Zagreb, 2005. The RBI innovations won two gold and two silver medals together with the special prize of the Association of Hungarian Inventors and the special prize of the International Salon des Inventions, Geneva, 2005.

OVERVIEW

The Ruđer Bošković Institute is the largest Croatian research centre for basic sciences, participating also in science applications and higher education. The multidisciplinary character of the Institute is reflected through the different research fields in physics, chemistry, oceanography (including marine and environmental research and geosciences), biology, biomedicine, computer science and electronics/engineering.

With an academic staff of 513, including 296 researchers, 189 Ph.D. students and 28 postdoctoral fellows, the RBI collaborates worldwide with many research institutions and universities.

The Ruđer Bošković Institute consists of twelve divisions, two centres, a library, as well as sections for maintenance, technical services and administration. The main bodies of the

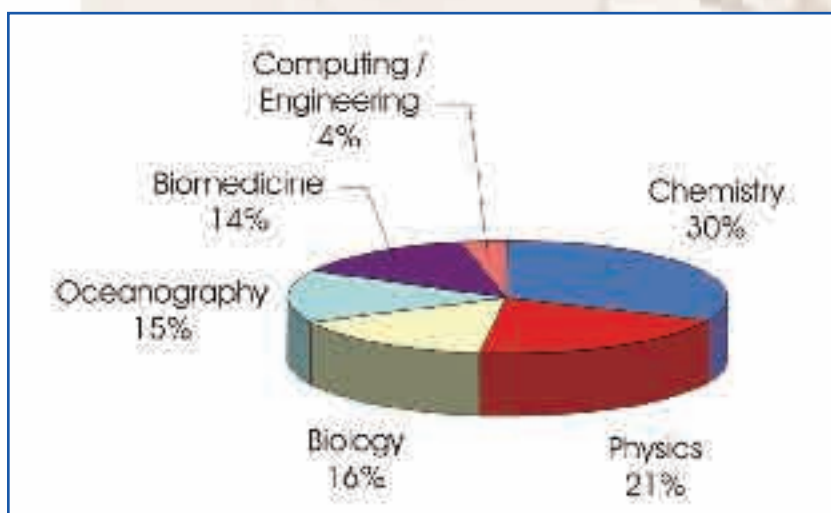


Figure 1. Composition of the academic staff at the RBI

Institute are the Board of Governors and the Scientific Council. Their organizational integration with the remainder of the Institute is displayed below (Figure 2).

ORGANIZATION OF THE INSTITUTE

Director: Mladen Žinić

Head of the Scientific Council:
Maja Osmak

Chairman of the Board of Governors:
Janko Herak

ACTIVITIES

Fundamental research

The total number of research articles published in 2004 was 578. Amongst these, 391 were published in journals cited by Current Contents. With less than 5% of the total number of scientists in the country working at the Institute, it is worthy of note that 27% of all Croatian articles in Current Contents journals originated from the RBI. A considerable proportion of these articles were published in high ranking journals.

Projects

The RBI has 125 projects in basic research

which are funded by the Ministry of Science, Education and Sport (MZOŠ). In August 2005 the three year project term ended. MZOŠ performed an evaluation of all the projects and, according to the results thereof, the financial support was continued at an increased, diminished or unchanged rate. A minority of unsuccessful projects were terminated. In addition to the fundamental projects, the Institute is involved in 65 international

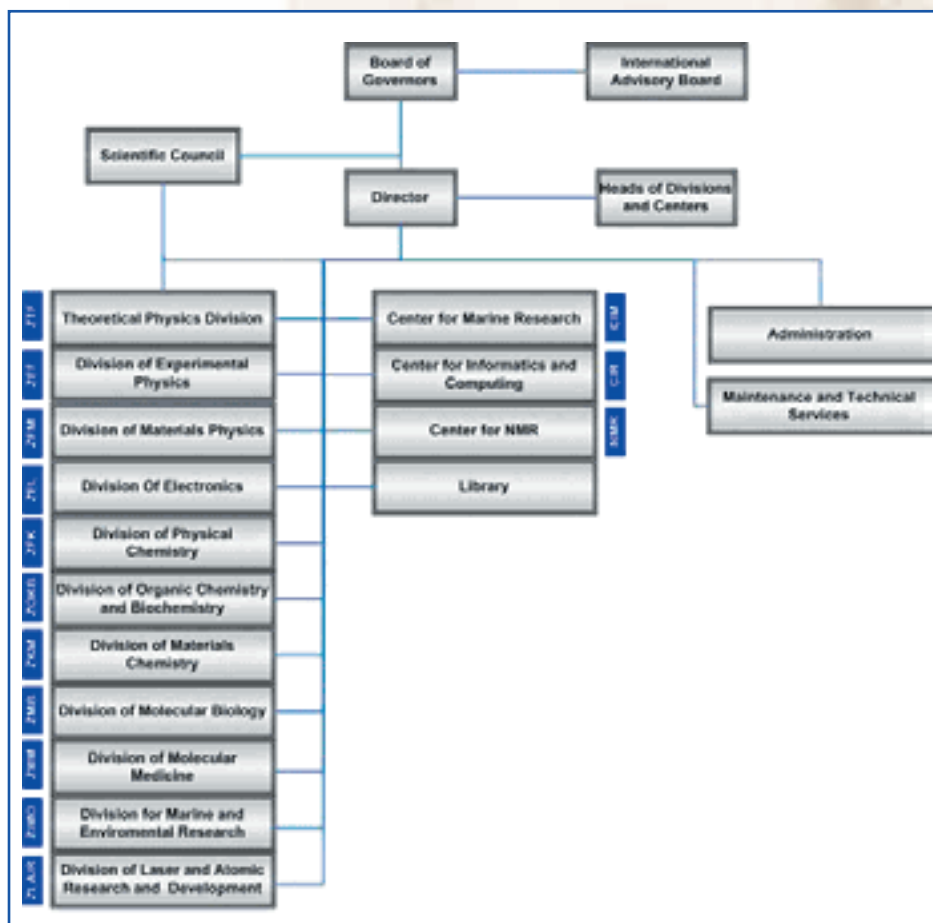


Figure 2. The organisational structure of the RBI

projects (38 bilateral, 2 FP5, 10 FP6, 11 IAEA, 2 COST, 1 INTERREG III, 1 UNESCO), as well as 11 applied and technological projects.

Higher education

In 2005, scientists from the Institute contributed 80 undergraduate courses and 180 graduate courses to the program of higher education in Croatia. Their respective distributions amongst the five universities at which they were conducted, as well as by the divisions and centres that contributed them are shown in Figures 3, 4, 5 and 6. In addition to the coursework, 48 B.Sc., 33 M.Sc. and Ph.D.

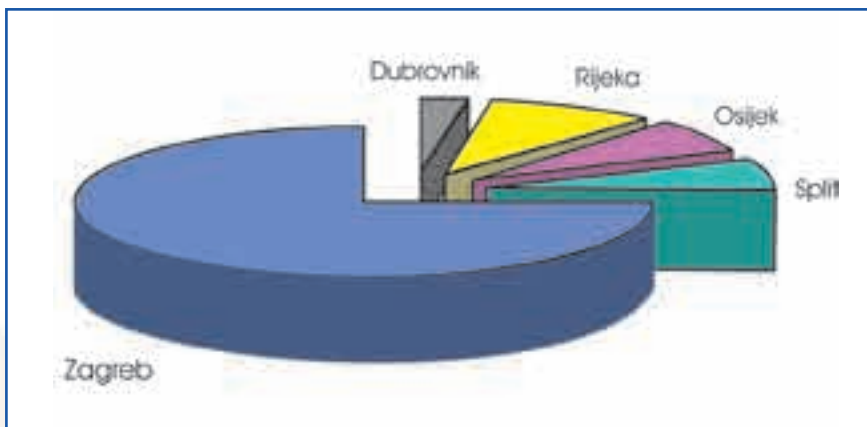


Figure 3. Distribution of the RBI held undergraduate courses (80) by domicile University.

theses were completed under the supervision of the RBI academic staff in 2005.

New instrumentation

In 2005 new high resolution Scanning Electron Microscope JEOL1 JSM-7000F was installed in Division of Materials Chemistry and put in operation.

This high performance and high sensitivity equipment, together with already available AFM and TEM, provide the basis for a more intensive approach to materials and nano-science at the RBI. In addition, the proteomic and genomic analysing system Bio Rad and Applied Biosystems Real Time PCR System arrived in the Division of Molecular

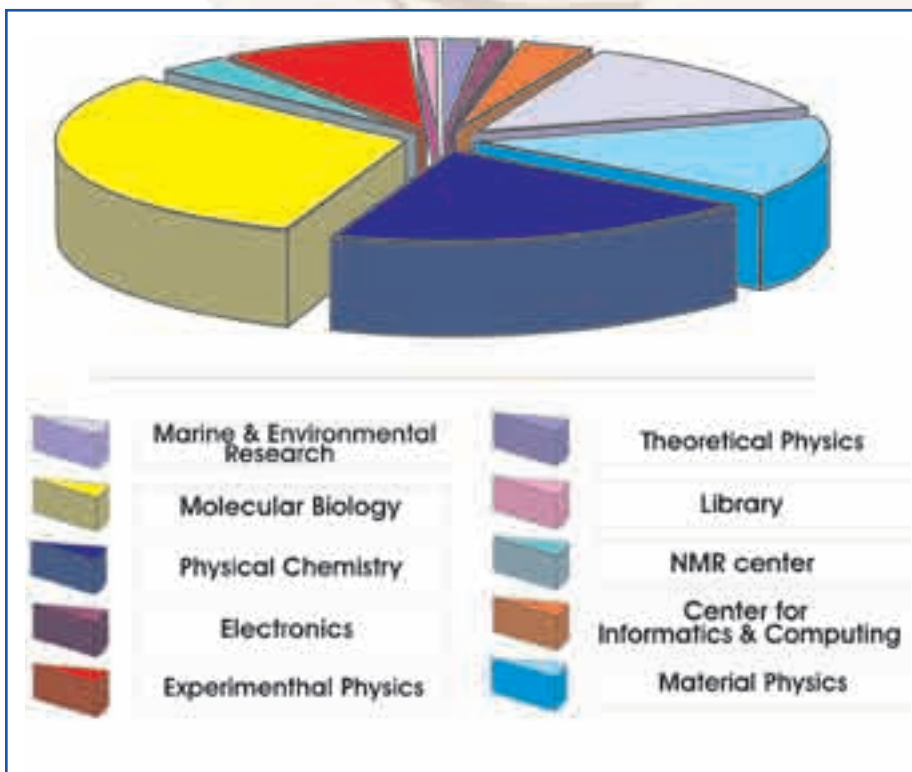


Figure 4. Distribution of the RBI-held undergraduate courses (80) by Divisions and Centres.

Medicine. Thanks to the combined financial support from the Ministry of Science Education and Sports and IAEA the new

Tandetron Accelerator was installed in the Department of Experimental Physics.

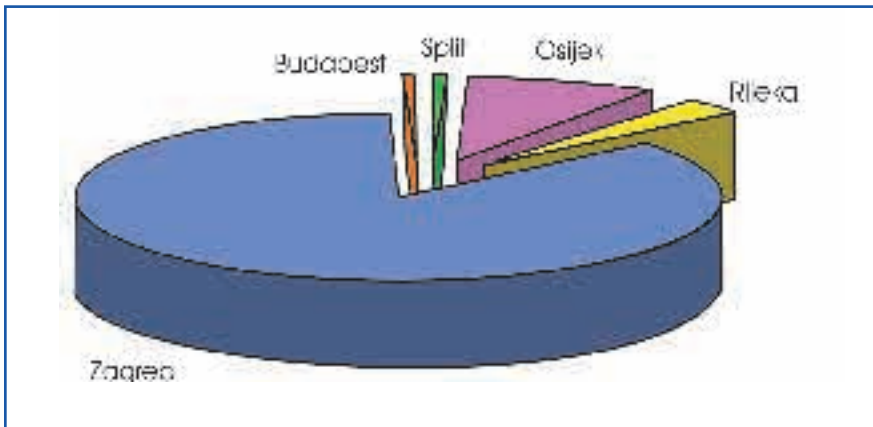


Figure 5. Distribution of the RBI held graduate courses (180) by domicile University

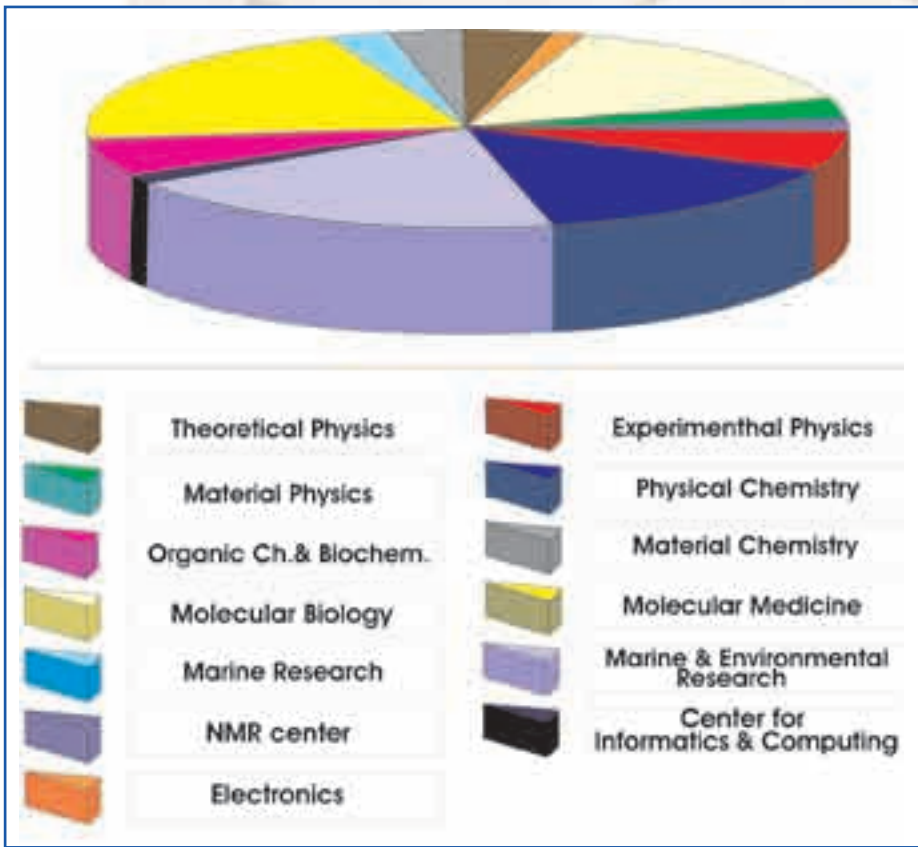


Figure 6. Distribution of the RBI held graduate courses (180) by Divisions and Centres

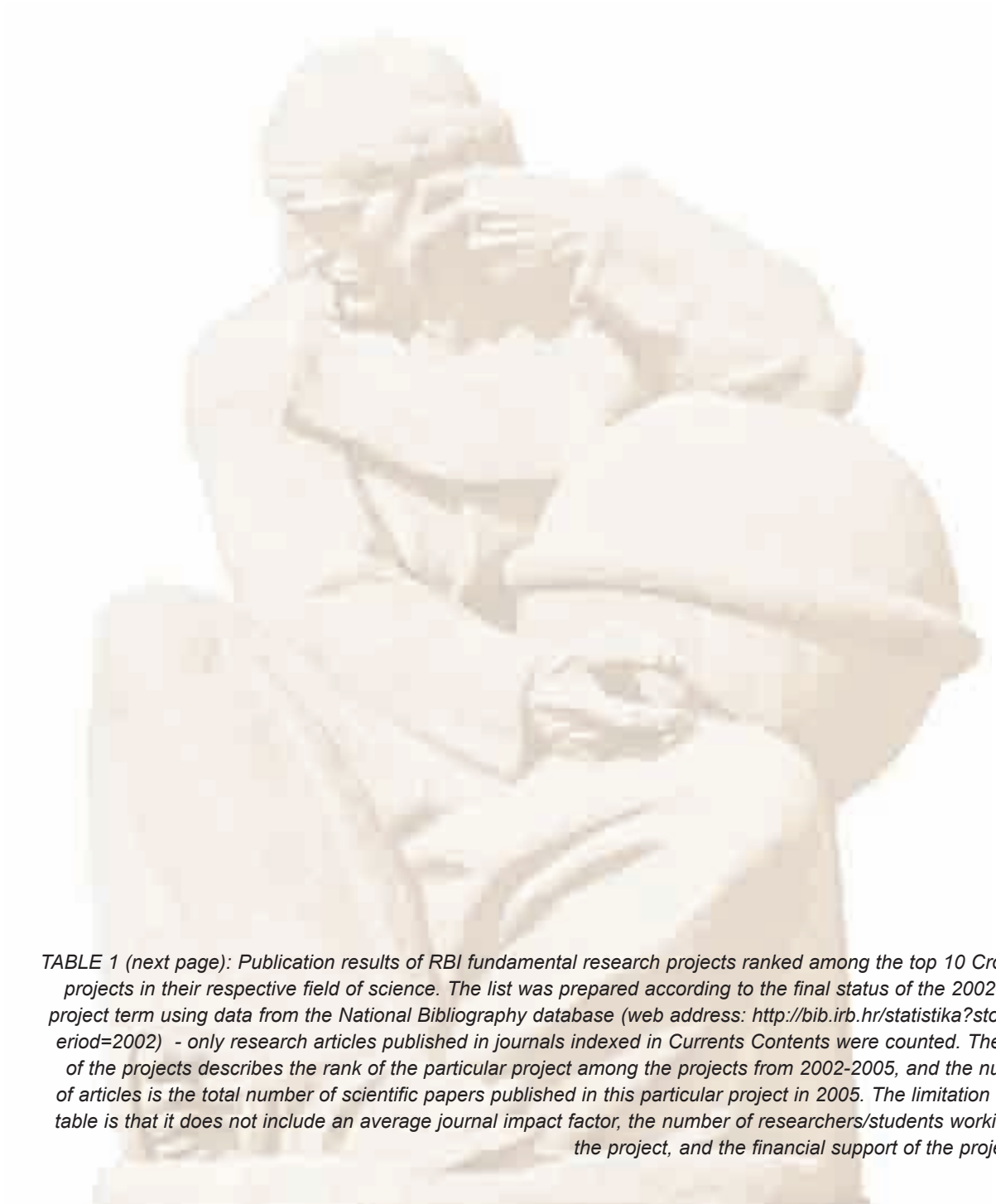
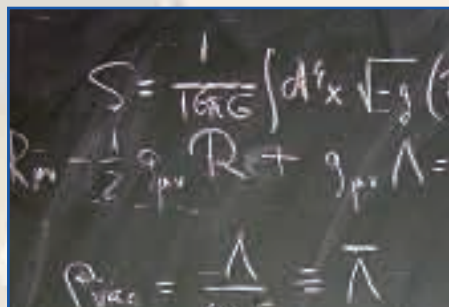


TABLE 1 (next page): Publication results of RBI fundamental research projects ranked among the top 10 Croatian projects in their respective field of science. The list was prepared according to the final status of the 2002-2005 project term using data from the National Bibliography database (web address: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

Field of Science - Number of National Projects in the Field	Project Title	Principal Investigator	Rank of the Project in the National Bibliography	Number of CC Articles Published in 2005
BIOLOGY - 60	Study of genes and genomes of evolutionary preserved and economically important organisms	Vera Gamulin	4	2
	Structure and function of plastids and cytoskeleton	Nikola Ljubešić	5	7
	Dynamics and genetics of bioactive molecules	Volker Magnus	6	3
	Cellular responses to physical, chemical and biological noxis	Maja Osmak	9	4
	Regulation of recombinant and recombinational repair	Mirjana Petranović	10	1
BIOMEDICINE - Neuroscience - 58	Neuropharmacology of serotonin system	Dorotea Mück-Šeler	1	3
	Molecular pathophysiology of serotonergic transmission	Branimir Jernej	4	4
	Oxidative/antioxidative status after treatment with opioids/opiates	Tatjana Marotti	8	2
BIOMEDICINE - Oncology - 73	Influence of gene/protein transduction on signalling pathways of transformed cells	Krešimir Pavelić	1	14
	Gene therapy of tumours by correction of tumour-suppressor genes	Jasminka Pavelić	2	10
	Oxidative stress and malignant disease	Neven Žarković	3	10
	Regulation of ectopeptidases and opoid receptors expression	Jelka Gabrilovac	8	5
	Modulation of immunological response by bioactive peptides	Biserka Pokrić	10	5
	Molecular genetics of gastrointestinal tumours	Sanja Kapitanović	10	4
CHEMISTRY - 75	Proton affinity and proton transfer reaction in chemistry	Zvonimir Maksić	1	14
	Reactivity and reaction mechanisms	Dunja Srzić	2	12
	Supramolecular organization in gels, molecular recognition and catalysis	Mladen Žinić	3	13
	Synthesis and microstructure of metal oxides and oxide glasses	Svetozar Musić	4	12
	Structure and dynamics of (bio)molecules	Biserka Kojić-Prodić	5	4
	Development and application of models in chemistry and bioinformatics	Nenad Trinajstić	6	5
	Reactive intermediates in resting and excited state	Mirjana Maksić	7	5
	Electron spin resonance in systems with paramagnetic particles	Boris Rakvin	8	9
	Stereoselective synthesis and catalysis	Zdenko Hameršak	10	3
GEOLOGY & OCEANOLOGY - 56	Mechanism of long-term changes of the Adriatic-sea ecosystem	Danilo Degobbi	1	13
	Programmed biosynthesis and genotoxic risk	Renato Batel	3	6
	Physics and biogeo-chemistry of trace metals in aquatic systems	Ivanka Pižeta	4	7
	Nature and reactivity of organic compounds in seawater and environment	Božena Čosović	5	7
	Geochemistry of recent and ancient sedimentation systems of the Adriatic platform	Goran Kniewald	6	7
	Research of the ebb and long-periodical dynamics of northern Adriatic	Milivoj Kuzmić	7	4
	Multidisciplinary sedimentological studies	Halka Bilinski	8	2
PHYSICS - 88	Fundamental interactions in physics of elementary particles and in cosmology	Branko Guberina	2	19
	Influence of defects and nanostructures on characteristics of semiconductors	Branko Pivac	3	10
	Heavy ion physics	Zoran Basrak	4	14
	Light atomic nuclei: clusters, nuclear molecules, reactions...	Đuro Miljanić	5	7
	Study of nanophase layers and nanocomposite hard electrolytes	Aleksandra Turković	6	8
	Quantum field theory, noncommutative spaces, and symmetries	Stjepan Meljanac	8	13
	Hadronic physics and QCD	Ivan Supek	9	9
	Physics and applications of nanostructures	Krešimir Furić	10	15
INFORMATION & COMPUTER TECHNOLOGY - 16	Automated knowledge discovery and reasoning	Nikola Bogunović	1	2

Theoretical Physics Division



<http://thphys.irb.hr>

DIVISIONAL ORGANISATION

Head: Branko Guberina

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

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

OVERVIEW OF THE DIVISION

The research performed in the Division is mainly concerned with the theoretical investigation of high-energy physics, such as particle physics, general and mathematical physics, astroparticle physics and cosmology. In addition, there is a substantial research activity in condensed matter physics. A special activity in the Division is the application of nonlinear dynamical analysis in biomedicine. In 2005, 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

Holographic dark energy

The generalized holographic dark energy model, in which the cosmological constant Λ and Newton's constant G_N are scale-dependent, has been used to set constraints on the renormalization-group (RG) evolution of both Λ and G_N . Assuming that ordinary matter scales canonically, it has been shown that the continuity equation fixes the infra-red (IR) cutoff, provided a law of variation for either Λ or G_N is known. Bringing a renormalization group running CC model, with a low energy scaling of CC given by quantum effects of particles with masses near the Planck mass, in full accordance with holography amounts to having an IR cutoff which scales as a square root of the Hubble parameter. It has been found that such a setup, in which the only undetermined input is the true ground state of the vacuum, yields a transient acceleration (B. Guberina et al., Phys Rev D 2005: 72: 125011). Furthermore, from the holographic dark energy requirement it

has been shown that, within quantum field theory in a curved background, the RG laws for Λ and G_N are completely determined in terms of the lowest part of the particle spectrum of an underlying field theory. One can then infer that the lowest-mass fields should have a Compton wavelength comparable with the size of the current Hubble horizon and, hence, holography actually brings us back to the quintessence proposal (B. Guberina et al., JCAP 2005: 0505: 001).

Noncommutative space-time

Gauge field theory on the kappa-deformed Minkowski spacetime has been analyzed using an expansion in a deformation parameter. It has been shown that the resulting effective action for U(1) gauge theory with fermionic matter expanded in ordinary fields is invariant under the action of the undeformed Poincare group (M. Dimitrijević et al., J High Energy Phys 2005: 0509: 068).

Two decay modes that are strictly forbidden in standard model (quarkonia decays into two photons and kaon decay into pion and photon) have been proposed as possible signatures of the space-time noncommutativity. An experimental discovery of $K \rightarrow \pi\gamma$ would indicate the violation of the Lorentz invariance, whereas a discovery of $J/\psi \rightarrow \gamma\gamma$ and/or $Y \rightarrow \gamma\gamma$ would indicate a violation of the Landau-Pomeranchuk-Yang theorem and a definitive appearance of new physics (B. Melić et al., Phys Rev D 2005: 72: 057502; Phys Rev D 2005: 72: 054004).

Solitons in the two-family Calogero model and matrix-model dualities

The two-family Calogero model has been examined by using the large-N collective field theory. The new paired soliton-antisoliton

solutions, localized at the same point, have been found (V. Bardek and S. Meljanac, *Europhys Lett* 2005: 72: 14). Duality between the real-symmetric and the quaternionic-real matrix model has been established using the collective-field approach. The $su(1,1)$ algebra, which generates dynamical symmetry of the matrix model, has made possible the construction of the master Hamiltonian in a conformally invariant way. This master Hamiltonian describes the dynamics of two collective fields, thus enabling the description of specific excitations of the hermitean matrix model (I. Andrić and D. Jurman, J High Energy Phys 2005: 0501: 039).

The van der Waals interaction and Density Functional Theory

The van der Waals attractive interaction is of great importance for a wide class of "soft matter" systems, including the physisorption of atoms on solid surfaces. Yet, because of its non-local character, it is difficult to integrate it into the Density Functional Theory calculations of the electronic structure, where the commonly used approximations are based on local and semi-local functionals (LDA and GGA). We have applied some recently developed schemes for incorporating the vdW interaction into the DFT on xenon atom monolayers adsorbed on Cu(111) and Pt(111) surfaces. We have found that the approach which treats the system as nearly isolated fragments gives excellent agreement with the observed structural and vibrational properties of the Xe adlayers, thus providing a first principles interpretation of the systems (P. Lazić et al., Phys Rev B 2005: 72: 245407).

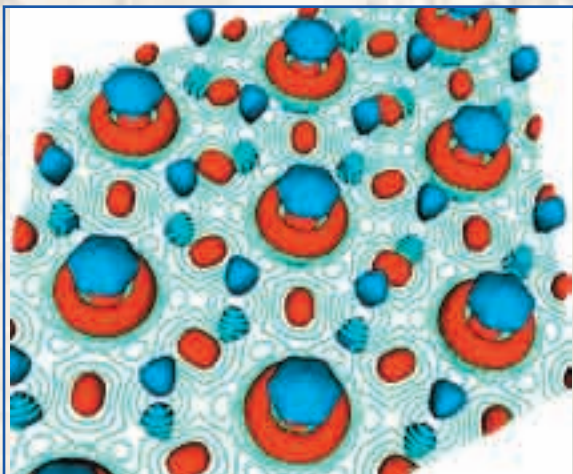


Figure 1: The redistribution of electronic density in an unsupported hexagonal xenon layer, calculated using the Density Functional Theory. Compared with isolated atoms, the charge accumulates in the plane of the atoms (red) at the expense of the outer regions (blue).

The Robin Hood approach to electrostatics

Embarking on a research project beyond their primary fields of interest, three young researchers have developed a new approach to the numerical calculation of problems

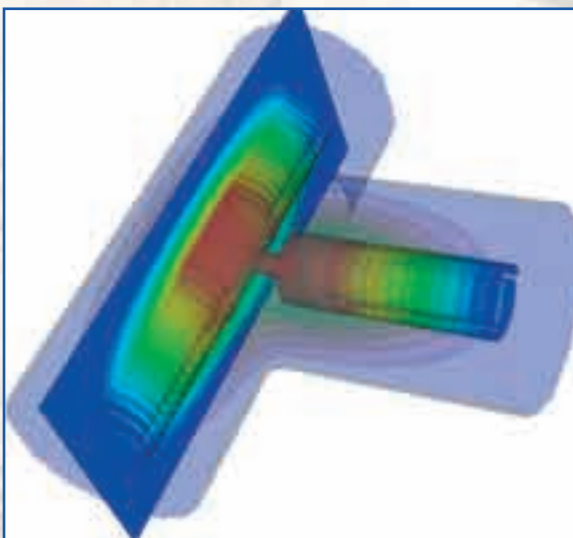


Figure 2: The potential inside the electrostatic Tandem Accelerator, calculated using the Robin Hood method. The maximum value of 1 MV is attained in the region denoted by red.

in electrostatics, based on the concept of nonlocal charge transfer. Their “Robin Hood” method has shown excellent properties in the calculations where it has been tested, surpassing the currently used methods in speed and accuracy (P. Lazić et al., J Comput Phys 2006: 213: 117).

Changes in multifractal properties for stable angina pectoris (SAP)

The multifractal approach has been applied to temporal fluctuations of heartbeat (RR) intervals, measured in various regimes of physical activity (ergometric data), taken from healthy subjects and those having stable angina pectoris (SAP). The problem we address here is whether SAP changes multifractality observed in healthy subjects. The G-moment method is used to analyse the multifractal spectrum. It is observed that both sets of data characterize multifractality, but a different trend in multifractal behavior is found for the SAP disease, under pronounced physical activity (A. Knežević et al., Physica A 2005: 358: 505).

PROJECTS

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

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

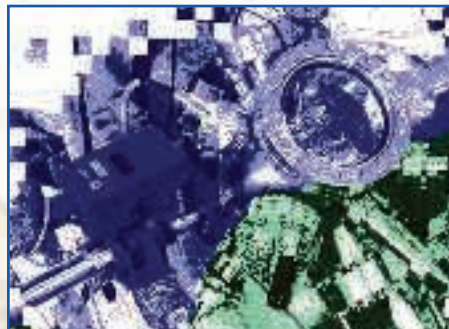
Collaborative projects:

1. Anđelka Andraši: Fundamental questions of nonabelian quantum gauge theories and cosmology, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Eötvös Loránd University, Budapest, Hungary
2. Neven Bilić, Scientific Joint Project: Investigations on the nature of Dark Matter and Dark Energy (DMDE) between the Particle Physics and Cosmology Group, Theoretical Physics Division of the Ruđer Bošković Institute and the Astrophysics Sector of the International School for Advanced Studies (SISSA), Trieste, Italy.
3. Branko Guberina, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and the Jozef Štefan Institute, Ljubljana, Slovenia, Hard-hadron physics in the standard model and beyond.
4. Kornelija Passek-Kumerički, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and the Institut für Theoretische Physik II, Ruhr-Universität Bochum, Germany, DFG project "Higher-order QCD corrections in exclusive processes-mesons and baryons".
5. Kornelija Passek-Kumerički, collaboration between the Ruđer Bošković Institute, Theoretical Physics Division and Institut für Theoretische Physik, Karl-Franzens Universität Graz, Austria, "Hard exclusive photo- and electroproduction of heavy quarkonia".

SELECTED PUBLICATIONS

1. Bilić N, Tupper G B, Viollier R D. Transient acceleration from a hybrid Chaplygin gas. *JCAP* 2005: 10: 003.
2. Guberina B, Horvat R, Nikolić H. Generalized holographic dark energy and the IR cutoff problem. *Phys. Rev. D* 2005: 72: 125011.
3. Guberina B, Horvat R, Štefančić H. Hint for Quintessence-like scalars from holographic dark energy. *JCAP* 2005: 0505: 001.
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5. Dimitrijević M, Jonke L, Möller L. U(1) gauge field theory on kappa-Minkowski space. *J. High Energy Phys.* 2005: 09: 068.
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7. Andrić I, Jurman D. Matrix-model dualities in the collective field formulation. *J. High Energy Phys.* 2005: 0501: 039.
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Division of Experimental Physics



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

DIVISIONAL ORGANISATION

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 IN 2005

The high intensity of basic research demonstrated in 2004 has been intensified in 2005 in all existing research projects. In addition to pushing forward old projects a number of new ones have been initiated. The high quality of research and a healthy and creative working atmosphere has stimulated the efforts of writing and submitting new proposals, and that has resulted in acquiring an enviable number of financially significant international research contracts. Applying the acquired knowledge to other areas has flourished and obligations taken in signing important international contracts have been realized according to the foreseen schedule.

TOP ACHIEVEMENTS

Measurement of forbidden eta decays

We have obtained two new and one improved upper limits on two rare and one forbidden η decays. At the 90% confidence level, we have obtained branching ratio $\Gamma(\eta \rightarrow 3\gamma) < 4 \times 10^{-5}$. This decay mode is forbidden by charge-conjugation invariance. We have also set the first upper limit on the doubly radiative, double π^0 decay $\Gamma(\eta \rightarrow \pi^0 \pi^0 \gamma \gamma) < 1.2 \times 10^{-3}$.

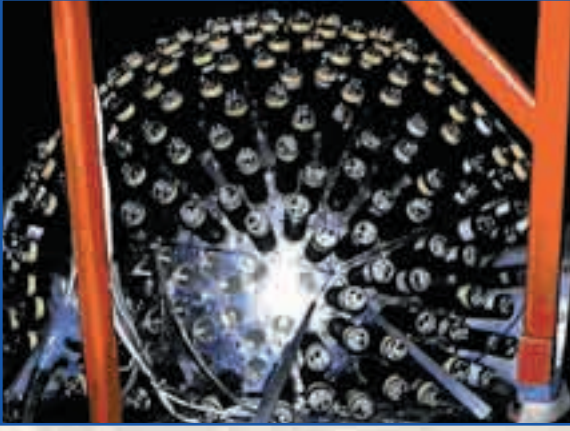


Figure 1: Crystal Ball segmented calorimeter

This decay is of interest as a special test of Chiral Perturbation Theory (χ PT) because of interesting mixture of anomaly-driven and G-parity violating amplitudes involved. We have not yet reached the level needed to test the theoretical models. Finally, no

candidates for the $\pi^0\gamma$ decay of the η have been identified. This decay mode is absolutely forbidden by conservation of angular momentum. Our result is $\Gamma(\eta \rightarrow \pi^0\gamma \rightarrow 3\gamma) < 9 \times 10^{-5}$. The results were obtained by using the Crystal Ball high-precision segmented calorimeter at the AGS and are based on the analysis of 28 million η mesons produced in the $\pi^-p \rightarrow \eta n$ reaction close to threshold.

Molecular states of ^{10}Be nucleus

The $^6\text{He}+^6\text{Li}$ and $^6\text{He}+^7\text{Li}$ reactions with three or more particles in the exit channel have been studied using a 18 MeV ^6He beam. Only the results on ^{10}Be nucleus are presented here as an illustration of all those obtained in the study. A very strong population and α -decay of the ^{10}Be state at 10.2

MeV have been observed, as well as the rare α -decay of the 2^+ state at 7.5 MeV. The most likely assignment for the 10.2 MeV state of 4^+ has been obtained from an angular correlation analysis of the data. All these results confirm our earlier suggestion that these two states together with the 0^+ state at 6.18 MeV are members of the same rotational band. Their large moments of inertia indicate a very special, molecular structure of ^{10}Be nucleus at the higher excitations (M. Milin et al., Nucl Phys A 2005: 753: 263).

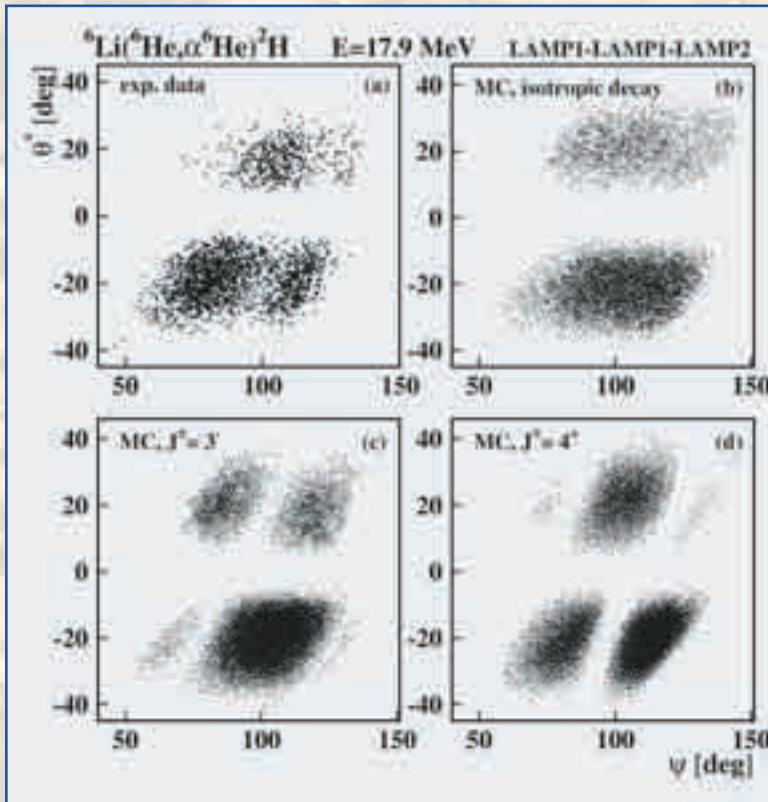


Figure 2 : Experimental data and the Monte Carlo simulations for the $^6\text{He}+$ decay of the ^{10}Be 10.2 MeV excited state populated in the $^6\text{He}+^6\text{Li}$ reaction

Search for solar axions

Axions, which are pseudoscalars that arise in models resolving the strong CP problem in quantum chromodynamics by the Peccei-Quinn mechanism, could also explain the mystery of dark matter in the Universe. At CERN, a group of scientists from the RBI Laboratory for Electromagnetic and Weak Interactions is involved in the CAST experiment, designed to search for solar axions. CAST has recently reported an upper limit on the axion-photon coupling of $1.16 \times 10^{-10} \text{ GeV}^{-1}$. This limit is comparable to the limit from energy-loss arguments on globular cluster stars and considerably more restrictive than any previous experiment over a broad range of axion masses. (K. Zioutas et al., Phys Rev Lett 2005: 94: 121301).



Figure 3: The CERN Axion Solar Telescope (CAST) experiment at CERN, which is looking for axions from the Sun. It uses a prototype magnet for the Large Hadron Collider combined with particle-physics detectors and X-ray techniques from space-born experiments.

Renormalization-group (Rg) running cosmologies and holographic dark energy

The procedure for phenomenological fixing of the RG scale is derived for cosmologies where the dark-matter component dilutes

canonically. Application of this procedure to the case where the RG evolution of the cosmological constant (CC) and Newton's constant is phrased within ordinary quantum field theory, shows remarkable consequences after merging with the concept of holographic dark energy. It is shown that such cosmological setup prefers two different contributions to the vacuum energy. Namely, besides a variable CC we show that an ultra-light scalar ("quintessence") is inevitable part of the particle spectrum.

Early energy transformation in heavy-ion reactions

A semi classical transport model study of the early reaction phase of nucleus-nucleus collisions has been carried out for a variety of system masses, asymmetries, and centralities at energies below 100 MeV/nucleon. It has been found that the maxima of the main forms of energy in the early compact reaction phase, namely, compression energy and heat (see Fig. 4), closely follow

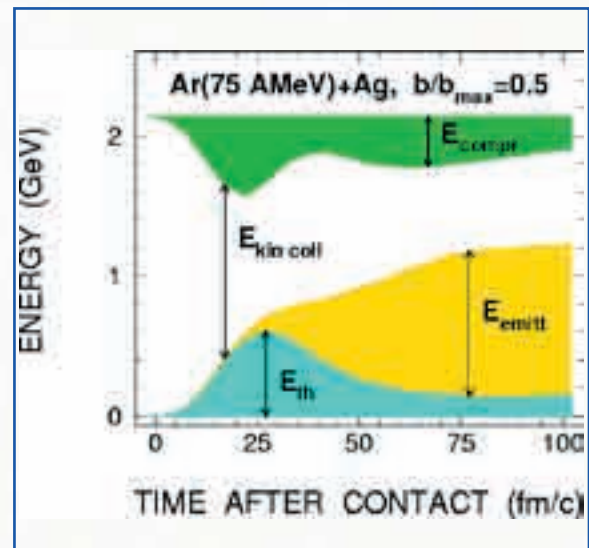


Figure 4: Time evolution of the energy components for the Ar + Ag reaction at 75 MeV/nucleon and an intermediate impact parameter.

the reaction geometry in the spirit of the participant–spectator picture with regard to the dependence on both reaction centrality and asymmetry. The role of elementary nucleon–nucleon collisions explains the *apparent controversy* of the quickly established local equilibrium throughout the compact system and complete lack of global equilibration.

New TOF ERDA/RBS beam line

A new Elastic Recoil Detection (ERDA) system based on micro channel plate (MCP) detectors and time-of-flight (TOF) detection set-up has been constructed in the Laboratory for ion beam interactions. The system is installed at the central beam line with a new spherical scattering chamber. This system will be dedicated for thin film characterization and depth profiling of light elements by forward scattering using heavy ion beams from a 6.0 MV tandem accelerator. Alternatively, the same detection system will be used at later stages with low energy ions from 1.0 MV tandem for low energy RBS analysis. Both techniques



Figure 5: TOF ERDA system at the central beam line of the Tandem Van de Graaff accelerator

should achieve depth resolution close to 1 nm near the sample surface. Sampling depth and depth resolution are determined by the choice of incident ions and energies and could be up to 1 μm .

Isotopic processes in environmental studies and radiocarbon dating

Water cycle and carbon exchange in nature have been investigated by monitoring of ^{14}C and ^3H isotopes in atmosphere, water and carbonate sediments. These studies were performed within the EU project ICA2-CT-2002-10009, a project signed with Plitvice Lakes National Park and a technical co-operation program with IAEA (CRO/8/006). The project has a special emphasis on the assessment of the anthropogenic influence on water resources in Lika, Dalmatia and Bihać region and eutrophication process in Plitvice Lakes. Absolute dating of artefacts from particular cultures and important historical objects, from Paleolithic to the Middle Ages in Croatia and Slovenia were performed within the co-operation with archaeological, paleontological and other scientific and cultural institutions.



Figure 6: Vacuum rig for benzene preparation for ^{14}C measurement by liquid scintillation counter

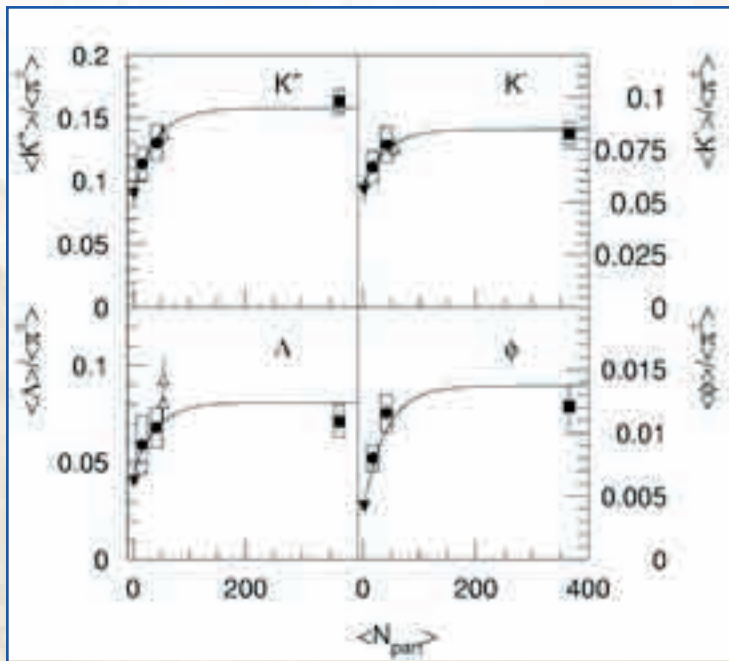


Figure 7: Experimental ratios of $\langle K^+ \rangle$, $\langle K^- \rangle$, $\langle \phi \rangle$, and $\langle \Lambda \rangle$ to $\langle \pi^\pm \rangle$ plotted as a function of number of participants $\langle N_{part} \rangle$.

Ultra-relativistic Heavy-Ion Collisions

Long range pseudo-rapidity correlations of oppositely charged particles were studied for p+p, C+C, and centrality selected Pb+Pb collisions at $\sqrt{s_{NN}} = 17.2$ GeV with the NA49 large acceptance detector at the CERN-SPS. A decrease of the Balance function with increasing system size and centrality could be related to an increasing delay of hadronization in central Pb+Pb collisions. Results are obtained on Ω and anti- Ω production in central Pb+Pb collisions at 40 and 158 AGeV beam energy. The yields are strongly under predicted by the string-hadronic UrQMD model and are in the better agreement with predictions from a hadron gas model.

In collaboration with "Mikrotrend", a Croatian electronics company, 130 pulsers were produced for the operation of the ALICE-TPC, and they will be

integrated with the electronics system of the LHC experiment ALICE. Our group has also developed an intelligent software package AFFAIR needed for the efficient performance monitoring of simultaneous running of thousands of computers and applications.

FP6 Project: EUROpean Illicit TRAfficking Countermeasures Kit (Euritrack)

Ten institutions from five countries have joined their efforts to develop, construct and test a European illicit trafficking countermeasures kit to non-intrusively detect explosives in shipping containers as well as other threatening or contraband materials such as drugs, chemical weapons and nuclear materials. The Neutron Laboratory of the Ruđer Bošković Institute has been chosen by all participants for the performance of laboratory tests that are needed for the project. This three year project is now in its second year and meeting all the milestones on time.



Figure 8: EURITRACK experimental set-up

PROJECTS

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

1. Hadronic physics and QCD, Ivan Supek
2. Light atomic nuclei: clusters, nuclear molecules, reactions ..., Đuro Miljanić
3. Interactions in subatomic and medical physics, Alfred Švarc
4. Heavy-ion physics, Zoran Basrak
5. Massive neutrinos and astro-particles, Ante Ljubičić
6. Photon-atom interactions and correlations, Tihomir Surić
7. Processes of fast ion interactions with matter, Milko Jakšić
8. Natural isotopes of weak activities and development of instrumentation, Bogomil Obelić
9. High-energy experimental physics, Krešo Kadija
10. Methods of explosive, chemical and nuclear material detection, Vladivoj Valković
11. Invariant special relativity and electrodynamics, Tomislav Ivezić

Other projects:

1. Remote experiments on accelerator (Milko Jakšić), MZOS Information Technology Project
2. Automatization of PIXE/RBS measurements (Ivančica Bogdanović Radović), MZOS Information Technology Project
3. EUROpean Nuclear Structure Integrated Infrastructure Initiative (EURONS) (Zoran Basrak), FP6 EU Project
4. Depth profiling of hydrogen and other light elements in thin films using ERDA spectroscopy (Ivančica Bogdanović Radović), bilateral project with Slovenia
5. Study of advantages and limitations of Si pin diodes as radiation detectors by ion beam

methods, bilateral project with Hungary

6. Measurements of differential cross sections for elastic scattering of ^1H and ^4He ions from selected light elements (Ivančica Bogdanović Radović), IAEA Research project
7. Utilisation of ion beam analysis and nuclear spectroscopy techniques in environmental and industrial applications (Milko Jakšić and Bogomil Obelić), IAEA Technical Co-operation project
8. Heavy ion acceleration in 1.0 and 6.0 MV electrostatic accelerators (Milko Jakšić), IAEA Research project
9. Upgrade of PIXE and STIM Imaging capabilities at Zagreb nuclear microprobe (Mladen Bogovac), IAEA Research project
10. Characterization of inorganic pigments used by selected painter(s) by nuclear microprobe (Stjepko Fazinić), IAEA Research project
11. Modification of electronic properties in insulators using nuclear microprobe (Zvonko Medunić), IAEA Research project
12. Study of anthropogenic pollution after the war and establishing the measures for protection of Plitvice National Park and Bihać region at the border area of Croatia and Bosnia-Herzegovina", European Commission, 5th Framework Programme, (Bogomil Obelić) ICA2-CT-2002-10009
13. Isotopic composition of atmospheric CO_2 as an indicator of atmospheric contamination (Ines Krajcar Bronić), Croatian-Slovenian joint research project
14. Investigation of influence of forest ecosystems of National Park Plitvice to the quality of water and lakes (Nada Horvatinčić), National Park Plitvice
15. Application of isotope techniques in investigation of water resources and water protection in the Karst area of Croatia. (Nada Horvatinčić), IAEA Technical co-operation programme

16. Inspection of shipping containers for undisclosed radioactive materials (Vladivoj Valković), IAEA Research contract
17. Control of illicit trafficking in threat materials and humans (Vladivoj Valković), NATO project
18. EURITRACK, European illicit trafficking countermeasures kit (Vladivoj Valković), EU FP6 Specific Targeted Research or Innovation Project
19. International collaboration between RBI and MAMI, University of Mainz, Germany on development of frozen spin polarization target (Ivan Supek).
20. International collaboration between RBI and University of Virginia, USA on PIBETA experiment (Ivan Supek)

EDUCATIONAL ACTIVITIES

A number of scientists from Division of Experimental Physics have continued to maintain a significant educational activity at undergraduate and graduate studies of University of Zagreb and University of Rijeka; the detailed list of courses is given elsewhere.

CONFERENCES ORGANIZED BY SCIENTISTS OF THE DIVISION

1. International Symposium on Utilization of Accelerators
Dubrovnik from 5th to 9th June 2005
2. International Workshop on Relativistic Heavy-Ion Physics/Physics with RPCs in FOPI Split at Adriatic coast from 25th to 29th May, 2005.
3. The 2nd International Workshop on Partial Wave Analysis ZAGREB2005
Zagreb, from 27th June to 2nd July.

INVITED LECTURES AT INTERNATIONAL CONFERENCES

1. T. Antičić, AFFAIR: a fast cluster and application monitoring software package, ROOT 2005 Workshop, Geneva, Switzerland.
2. Z. Basrak, The early-reaction-phase dynamics of heavy-ion collisions below 100 MeV/u International Workshop on Multifragmentation and Related Topics, Catania, Italy
3. N. Horvatinčić (with A. Gokgoz, M. Akgun), Yenice travertines, Kamara hot spring fissure ridge and Guney waterfall tufa, International Travertines Symposium, Travertines of Denizli basin, Western Turkey
4. K. Kadija, Exotic Cascades at NA49, Cracow Epiphany Conference on Hadron Spectroscopy, Cracow, Poland
5. S. Szilner, Multinucleon transfer reactions studied with the PRISMA magnetic spectrometer, International Conference on Frontiers in Nuclear Structure, Astrophysics and Reactions, Aegean island of Kos, Greece.
6. T. Surić, Correlation effects in high energy photoabsorption and in Compton scattering, 20th International Conference, X-Ray and Inner-Shell Processes, Melbourne, Australia
7. A. Švarc, The importance of inelastic channels in eliminating continuum ambiguities in pion-nucleon partial wave analyses, Plenary talk at International Workshop on the Physics of Excited Baryons (NSTAR 05), Tallahassee, Florida, 10-15 Oct 2005.
8. V. Valković, Applications of nuclear techniques relevant for civil security, Europhysics Conference on New Trends in Nuclear Physics, Applications and Technologies, NPDC19 Pavia, Italy.

SELECTED PUBLICATIONS

1. Andronić A, et al. (RBI-FOPI collaboration: Basrak Z, Čaplar R, Gašparić I, Korolija M). Excitation function of elliptic flow in Au+Au collisions and nuclear matter equation of state. Phys Lett B 2005: 612: 173.
2. Alt C, et al. (NA49 Collaboration-IRB: Anticic T, Kadija K, Šuša T). Omega- and anti-Omega+ production in central Pb+Pb collisions at 40 and 158 A GeV. Phys Rev Lett 2005: 94: 192301.
3. Babić A, Guberina B, Horvat R. Stefančić H. Renormalization-group running cosmologies: a scale-setting procedure. Phys Rev D 2005: 71:124041.
4. Bogdanović Radović I, Medunić Z, Jakšić M, Siketić Z, Skukan N. Ion-induced electron emission ERDA with a nuclear microprobe. Nucl Instr Meth B 2005: 231: 123.
5. Milin M, Zadro M, Cherubini S, Davinson T, Di Pietro A, Figuera P, Miljanić, Đ, Musumarra A, Ninane A, Ostrowski AN, Pellegriti MG, Shotter AC, Soić N, Spitaleri C. Sequential decay reactions induced by a 18 MeV ^6He beam on ^6Li and ^7Li . Nucl Phys A 2005: 753: 263.
6. Nefkens B.M.K., et al. (Marušić A., Supek I.) Test of charge conjugation invariance. Phys Rev Lett 2005: 94: 041601.
7. Surić M, Juračić M, Horvatinčić N, Krajcar Bronić I. Late Pleistocene - Holocene sea-level rise and the pattern of coastal karst inundation - records from submerged speleothems along the Eastern Adriatic Coast (Croatia). Marine Geology 2005: 214 163.
8. Vjesti G, Pesente S, Nebbia G, Lunardon M, Sudac D, Nađ K, Blagus S, Valković V. Detection of hidden explosives by using tagged neutron beams: status and perspectives. Nucl Instr Meth Phys Res B 2005: 241: 748.
9. Zioutas K, et al. (Lakić B., Krčmar M., Ljubičić A.). First results from the CERN axion solar telescope. Phys Rev Lett 2005: 94: 121301.

Division of Materials Physics



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

DEPARTMENT ORGANISATION

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 IN 2005

The research in the Division of Materials Physics is focused on fundamental and applied studies of physical parameters and processes which describe and connect the microscopic, mesoscopic and macroscopic properties of condensed matter and molecules. Certain aspects, such as the mutual interactions of defects, their impact on the relation between microscopic and macroscopic properties of materials, as well as nanophase and glassy material characteristics, prove particularly important. The methods of investigation include the study of amorphous and nanocrystalline thin films produced by thermodynamically non-equilibrium processing (magnetron sputtering, ion implantation), particularly Al-based amor-

phous alloys, and a-Si and a-Si_{1-x}C_x:H films. Various types of nanostructured materials have been produced and examined by different methods: nanolaminates of semiconductor (Ge, Si)/ dielectric (SiO₂) bilayers - as precursors for nanoparticles, multilayer α -W/ β -W, and nanocrystalline metals (nc-Ni). The Division is also involved in fundamental research in the field of molecular and solid state physics with special emphasis on vibrational spectroscopy. The systems under investigation vary in their origin and composition from metals, semiconductors, and ceramics on one side, to molecular crystals and biological samples on the other. Finally, optical interactions in matter as well as spontaneous and induced self organization in condensed systems are the subject of intensive research. In 2005, scientists from the Division published 41 papers in journals listed in Current Contents with an average impact factor of 1.41.

TOP ACHIEVEMENTS

Nanosciences

Nanoscience and/or nanotechnology has been the most active direction of both fundamental scientific research and developments in technology for the Division of Materials Physics. The Croatian Nanonetwork "Nanosciences: a road to new technologies",

coordinated by M. Milun (Institute of Physics) has successfully completed a two-year term by submitting a Final Report at the end of 2005. From 22 domestic projects, those from the Division of Material Physics, lead by B. Pivac, N. Radić, D. Gracin and A. Turković, showed the greatest extent of cooperation resulting in the CC publications

Selected results in the study of radiation defects in semiconductors

Electrically active defects induced by neutron irradiation in n-type Czochralski-grown (Cz) Si crystals have been studied by means of capacitance transient techniques. Four electron traps were observed after neutron irradiation in phosphorus-doped Cz Si crystals. One of the most interesting features is a dominating asymmetric peak with its maximum at around 220 K and an activation energy for electron emission of 0.42 eV. From the annealing behaviour, by use of high-resolution Laplace DLTS, it was revealed that while some of these defects anneal out, others act as sources of vacancies as evidenced by an increase in the concentration of vacancy–oxygen

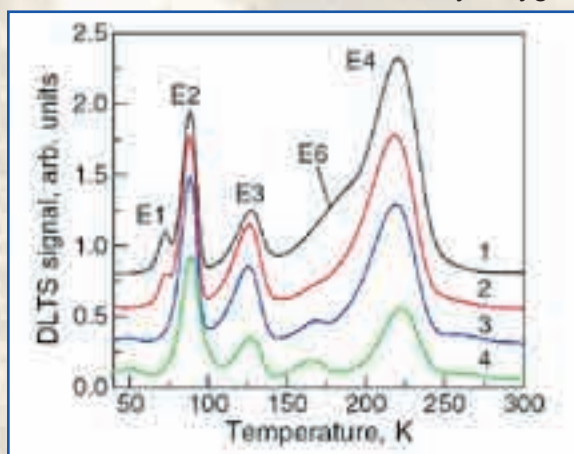


Figure 1: Development of DLTS spectra for a neutron irradiated Cz Si:P sample upon 60 min isochronal annealing with temperature increments of 50°C from 100°C (1 > 4).

pair (VO), and the divacancy (V2). It is suggested that some of the defects contributing to the E(0.42) peak are related to the small vacancy clusters (I. Kovačević et al., J Phys Cond Matter 2005: 17: S2229).

Structural properties of vanadium/cerium oxide thin films

It is shown that the particle scattering model, used in analyzing the data from GISAXS measurements, can be applied for estimation of the structural properties of the vanadium/cerium oxide thin films as well as for following their structural modifications in the process of lithium intercalation. Since the SAXS analysis is model-dependent and suffers from the influence of various material properties, two-dimensional detection of the scattering signal is applied and the results are compared to those of the AFM surface imaging. It was concluded that the observed aspects of the GISAXS intensity maps supported by the AFM analysis provide a contribution to the modelling of nanostructured intercalation electrodes (M. Lučić-Lavčević et al., J Chem Inf Mode 2005: 45: 1553).

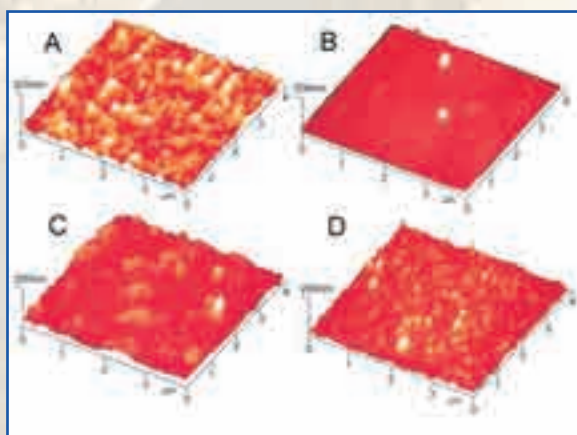


Figure 2: AFM micrographs for V_2O_5 , V/Ce oxide at 38% of V (samples A and B) and the same ones Li^+ intercalated (samples C and D).

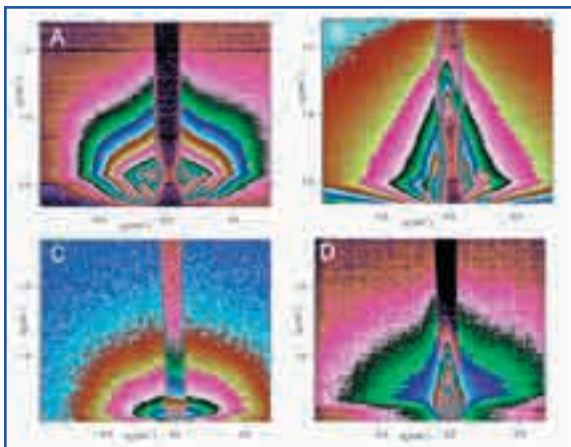


Figure 3: GISAXS 2-D patterns from V oxides (left samples A and C) and V/Ce oxides (right, samples B and D), non-intercalated (top) and Li intercalated (bottom).

Installation of a new cryostat

The new CCS 350 cryostat (Figure 4) enables cooling of the sample to temperatures as low as 8 K. Presently matrix isolation of acetylacetone in argon is under way.



Figure 4: New optical cryostat from JANIS installed in Molecular Physics Laboratory.

Silicon nanostructures

Nanocrystalline silicon exhibits a strong emission in the visible spectral region depending on the size of nanocrystals. Moreover, the recent discovery of optical gain in silicon nanocrystals embedded in silica matrix promises the imminent fabrication of a silicon laser. The structural and optical

properties of silicon nanocrystals, prepared by the LPCVD and PVD methods and by HF electrochemical etching, were investigated by the Raman, IR and SEM techniques, as well as electrical measurements. The possibility of optical gain was examined by the so called VSL technique.

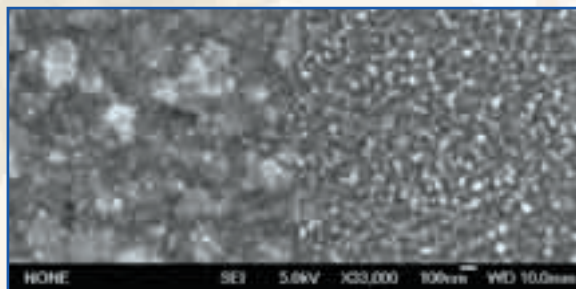


Figure 5: The effects of the LPCVD reactor temperature on the morphology of the silicon nanoparticles.

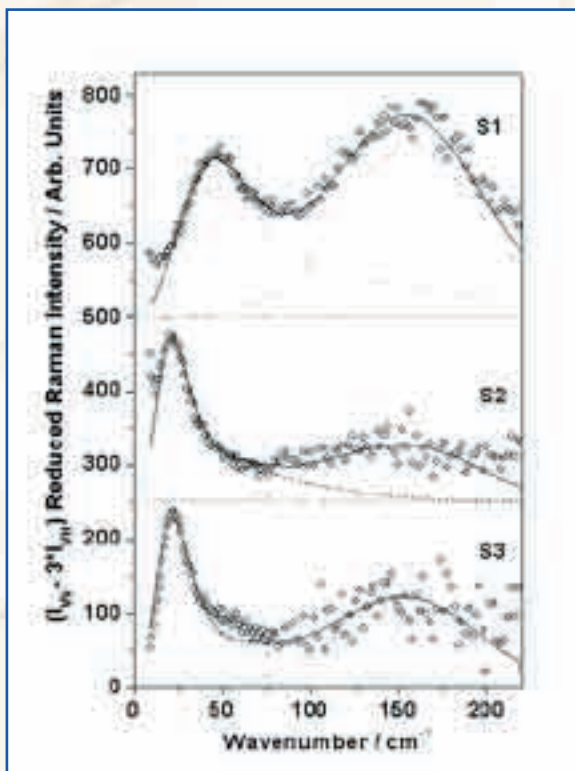


Figure 6: A low frequency Raman scattering technique as a tool for determination of size distribution of silicon nanoparticles prepared by PVD.

Generation of nonlinear surface waves by nanosecond laser pulse

The evolution of nonlinear waves in nanosecond laser-matter interaction with an indium target was studied as a function of the laser energy density (E_s) of a Nd:YAG laser. The illustrations in Figure 7 from a) (3.75 J/cm^2) to f) (5 J/cm^2) are evidence that the evolution of deep nonlinear waves on the melted In layer starts by the formation of shallow capillary waves, which play the role of a precursor at 3.75 J/cm^2 . At $E_s \sim 5 \text{ J/cm}^2$ the strength of deep fluid waves grows to a critical stage, when the break-up occurs.

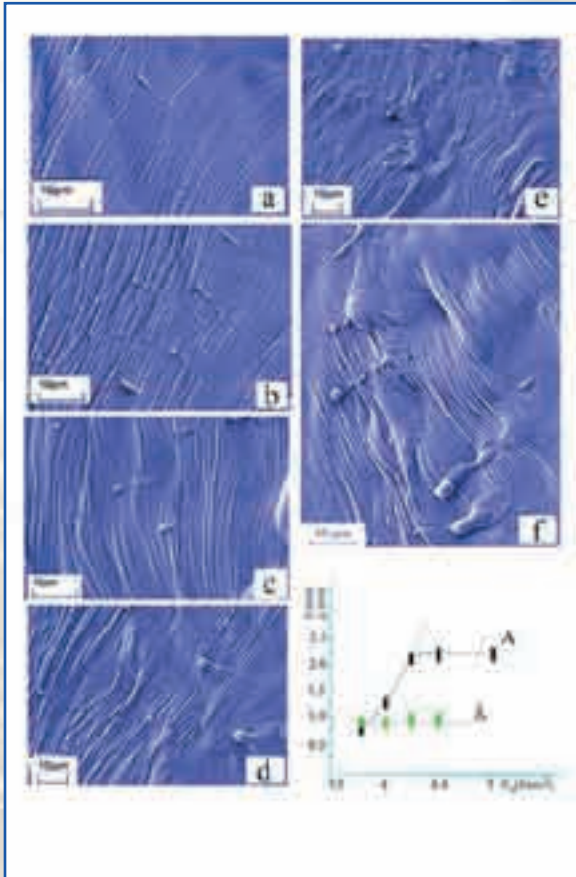


Figure 7: Evolution of the nonlinear waves with energy density from small capillary waves (a) to the deep nonlinear waves (d), which transform into breaking waves (f). Lower right: Corresponding diagram of the amplitude and the wavelength with energy density. Material: Indium.

The holes following the largest crests of the breaking waves are very deep and clearly seen. The corresponding diagram (Figure 7: lower right) shows the amplitude A and the wavelength λ of the capillary waves as the function of the energy density; the wavelength λ is almost constant in the range of E_s from 3.75 J/cm^2 to 5 J/cm^2 , while the amplitude A grows exponentially from 0.8 mm (at 3.75 J/cm^2) to $\sim 2.2 \text{ mm}$ (at 4.25 J/cm^2), as the maximal value (S. Lugomer and J.N. Zabusky, Appl Phys Lett 2005: 87: 204101).

Conference organized by the DMP scientists

The 12th International Meeting "Vacuum Science and Technique", Trakošćan, May 18, 2005, was organized by the Division members N. Radić, B. Pivac, I. Kovačević and T. Car on behalf of the Croatian Vacuum Society. The attendance was 63 participants and several exhibitors, and the Book of Abstracts was published.



PROJECTS

Projects supported by the Ministry of Science, Education and Sport

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

Research and development projects

1. Stress in thin films, N. Radić, (Bilateral collaboration with Slovenia)
2. Study of nanocomposite polymer electrolytes, A. Turković, (Bilateral collaboration with Slovenia)
3. Study of disordered materials, nano-optical layers, M. Ivanda, (Bilateral collaboration with Slovenia)
4. Chemically durable iron phosphate glasses for vitrifying stimulated nuclear waste, A. Moguš-Milanković, (IAEA)

5. Hybrid photovoltaic module, D. Gracin (Ministry of Science, Education and Sport-HITRA-STIRP Project TP-02/0098-35)
6. LPMAS, D. Gracin (EU- FW6 -INCO-Project No FP6-509178)
7. RISE, U.V. Desnica (EU-FW6-INCO-Project No FP6-509161)
8. Istraživanje silicijevih i germanijevih nanostrukture, B. Pivac (COGITO - Bilateral collaboration with France)

Invited lectures

Dubček, Pavo: Structure of ion beam synthesized II-VI nanocrystals. Semiconductor Nanocrystals 2005, Budapest, Hungary, 10-12 September 2005

SELECTED PUBLICATIONS

1. Lugomer S, Zabusky JN.: Nonlinear and breaking micron waves at the edge of laser-liquefied metal pool. Appl Phys Lett 2005: 87: 204101
2. Lučić-Lavčević M, Dubček P, Crnjak-Orel Z, Turković A.: GISAXS View of Vanadium Cerium Oxide Thin Films and Influence of Lithium Intercalation. J Chem Inf Mode 2005: 45: 1553
3. Kozarac Z, Risović D, Frka S, Möbius D.: Reflection of light from the air/water interface covered with sea-surface microlayers. Marine Chem 2005: 96: 99
4. Lugomer S, Mihaljević B, Peto G, Toth A, Horvath E.: Sponge-like Metal Surface Generated by Laser in the Semiconfined Configuration. J Appl Phys 2005: 97: 073305

5. Švrček, V.; Rehspringer, J.L.; Slaoui, A.; Pivac, B; Muller, J.-C.: Clustering/ declustering of silicon nanocrystals in spin-on glass solutions. *Semicond Sci Tech* 2005: 20: 314
6. Kovačević I, Markevich VP, Hawkins ID, Pivac B, Peaker AR.: Vacancy-related complexes in neutron-irradiated silicon. *J Phys Cond Matter* 2005: 17: S2229
7. Mohaček Grošev V.: Spectroscopic arguments for a new crystal phase of glycolaldehyde. *J Raman Spectr* 2005: 36: 453
8. Risović D, Furić K.: Comparison of Raman spectroscopy methods for determination of super-cooled and liquid water temperature. *J Raman Spectr* 2005: 36: 771

Division of Laser and Atomic Research and Development



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

LAIR

DIVISIONAL ORGANISATION

Head: Hrvoje Zorc

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

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

OVERVIEW OF THE DIVISION

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

In the medical field, emphasis is placed upon the development of new instrumentation, in particular that relevant to technologies and techniques for photodynamic diagnostics and therapy of skin malignant diseases. Considerable attention is also paid to the implementation of our instrumen-

tation in a clinical setting. This activity, in co-operation with clinics, results in interactive development as well as in optimization of diagnostics and therapy instrumentation and procedures.

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

TOP ACHIEVEMENTS

Design of optical filters

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

MediLED 5

The major achievement in 2005 was development and testing of an advanced apparatus for photodynamic diagnosis and therapy (PDT and PDD) of skin malignant diseases under the brand name - "MediLED 5". This device will soon be installed in the "Clinical hospital Centre Zagreb" ("CHC Zagreb") where the pre-clinical testing will be performed followed by its further clinical implementation and diagnosis/therapy protocol optimization, according to the contract signed between "Ruđer Bošković Institute" and the "CHC Zagreb" authorities.



Figure 1: "MediLED 5" illuminator for PDT/PDD will be soon implemented in the "CHC Zagreb" and «CH Split».

Night vision

Besides the optical and medical program, the division continued with a project for the development of devices for night and/or low visibility monitoring. The new apparatus is based on the last (IV) generation of image intensifier tube. Preliminary testing in night conditions has been performed.

PROJECTS

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

1. Photonics of imaging and non-imaging optical systems, Hrvoje Zorc (0098140)

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

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

Own research and development projects

1. Development of night monitoring systems
2. Contract with the Ministry of defence - final phase

Patents

In 2005, international patent submissions (initially submitted in 2004.) were advanced to the next phase in the patent recognition process.

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

Awards

In 2005, the Division received the award for the new device developed through Ministry of Science Education and Sports project - HITRA-TEST. At the ARCA - international exhibition of inventions, held in Zagreb, our apparatus "MediLED 5" received the Silver Arca award for the most inventive products.



Figure 2: Received Silver Arca award for the "MediLED 5" apparatus, at 3rd ARCA inventions exhibition, held in Zagreb in September 2005.

Selected publications:

1. Janicki V, Wilbrandt S, Stenzel O, Gabler D, Kaiser N, Tikhonravov A, Trubetskov M, Amotchkina T. Hybrid optical coating design for omnidirectional antireflection purposes. J Optics A: Pure Appl Optics 2005;7: L9.
2. Kovačević I, Dubček P, Zorc H, Radić N, Pivac B, Bernstorff S. GISAXS characterization of Ge islands on Si (100) substrates. Vacuum 2005: 80: 69.
3. Janicki V, Lappschies M, Gortz B, Ristau D, Schallenberg U, Stenzel O, Kaiser N. Comparison of gradient index and classical designs of a narrow band notch filter. Proceedings of SPIE 2005: 5963: 60.
4. Janicki V, Leitel R, Wilbrandt S, Stenzel O, Gabler D, Kaiser N. Design of hybrid coatings composed of homogeneous layers and refractive index gradients. Proceedings of SPIE 2005: 5963: 49.
5. Pivac B, Kovačević I, Dubček P, Zorc H, Radić N, Bernstorff S. Grazing-incident small-angle X-ray scattering (GISAXS) study of SiO/SiO₂ superlattice. Proceedings of the First International Workshop on Semiconductor Nanocrystals, SEMINANO 2005: 1 In: Podor B, Horvath ZJ, Basa P (eds.). Budapest : Hungarian Academy of Sciences, 2005. 144.



Division of Electronics



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

DIVISIONAL ORGANISATION

Head: Tomislav Šmuc

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

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

OVERVIEW OF THE DIVISION

The Division of Electronics continues to work on research and development of novel intelligent data and signals analysis techniques and algorithms for applications in areas of high scientific interest. In particular, priority is given to the fields of biomedicine, computational biology and bioinformatics, as well as on applications in the field of real-world signal measurements and processing. With new data acquisition equipment and information processing tools, the division continued to develop common infrastructure for tackling complex scientific and technological problems related to knowledge discovery, pattern recognition and modeling of different sources of data and signals. This was also a year of intense collaboration with

scientists from different bio-science fields in focusing on challenging inter-disciplinary problems.

TOP ACHIEVEMENTS

Machine learning and data mining research and applications

A new approach for insightful data analysis, based on iterative application of subgroup discovery methodology enables detection of the general properties of the target concept, its characteristic subpopulations, and generation of classification descriptions of the target class. The methodology has been successfully applied in the brain ischemia domain and for the analysis of the political instability concepts from the state failure dataset.

A novel classification tool MIFS/SVM, coupling an advanced feature selection technique with a support vector machine classification algorithm was successfully applied to gene micro-array expression data related to the problem of discriminating between two different leukemia types.

In collaboration with Centre for Informatics and Computing, a well known machine learning algorithm Random ForestTM, was completely rewritten and enhanced with a number of new features, and enabled to work on parallel computing platforms.

Applications in bioinformatics and computational biology

Work on sequence indexing, data retrieval and data compression algorithms is extended to include free text compression and DNA sequences indexing algorithms. Adaptive features of previously developed algorithms are used in the compact indexing structures development (S. Ristov, Software: Practice & Experience 2005: 35: 445). Preliminary research was done on classification of unknown proteins to gene ontology functional groups using a novel amino-acid sequence feature representation. Application of machine learning techniques for in-silico screening and quantitative structure activity relationship modeling was also tackled in cooperation with collaborators from molecular medicine and physical chemistry laboratories of the Institute (F. Supek et al, Period Biol 2005: 107: 451).

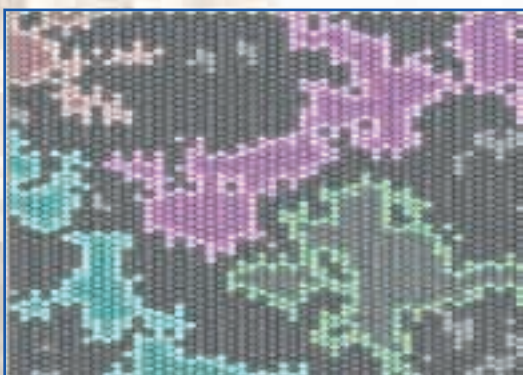


Figure 1: Self-organizing-map graph of 10000 drug-like compounds based on 50 molecular descriptors. Distinct colours of 'compound islands' on the map reflect their cytotostatic activity (GI50 values) on SW-620 colon cancer cell line.

Complex measurement systems:

Research and development of short time interval measurement methods have been continued with application to measurements and statistical analysis of stochastic pulse

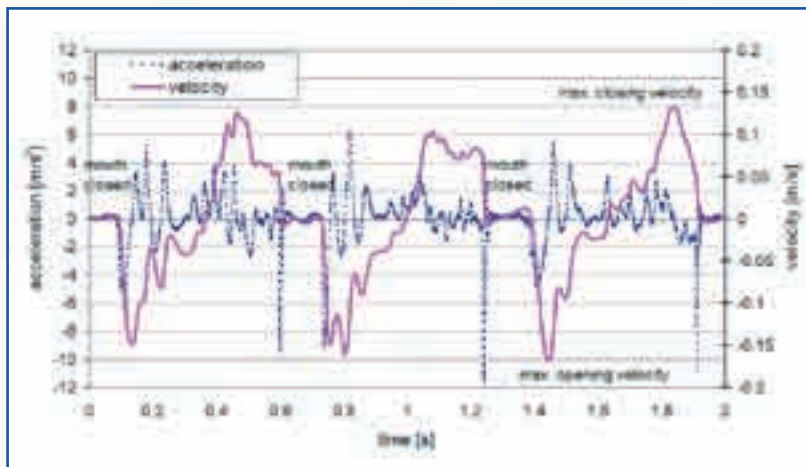


Figure 2: Human jaw kinematics measured with G-LINK wireless acceleration measurement system.

generator timing characteristics. One of the main applications of such generator is in the research and development of new methods for random bit generation. This work is also important for generation of information impulse carrier in "Ultra-Wide Band" communication systems.

Highly accurate measurements of natural gas flow require implementation of complex mathematical model for isentropic expansion of gas. The corresponding analytical procedure for the calculation of the isentropic exponent, based on natural gas extended virial type characterization equation, was derived. Simulated measurements show considerable effect of the isentropic expansion to the accuracy of flow-rate measurements (I. Marić et al., Flow Measur Instrum 2005: 16: 13).



Figure 3: QRBG121 – Quantum random number generator, a fast non-deterministic random number generator with bit rate of 12Mb/s. The prototype was awarded a gold medal by International Salon des Inventions, Geneve, 2005.

PROJECTS

Projects supported by the Ministry of Science Education and Sport (MZOS)

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

International projects, bilateral and multilateral collaborations

1. NATO Security Through Science project: Advanced Data- and Knowledge-Driven Methods for State Failure Risk Assessment, in collaboration with University of Ulster, United Kingdom and University of Seville, Spain.
2. Joint Croatian-Slovenian project: Intelligent Data Analysis, in collaboration with J.Stefan Institute, Ljubljana, Slovenia.
3. Joint Croatian-French project: Intelligent Data Analysis for Decision with Applications in Medicine, in collaboration with University of Lyon, France,

IRISA, Rennes, France, and University of Zagreb, Croatia.

HEARTFAID – EU sixth framework project

Laboratory for information systems has been engaged in preparation of the STREP project HEARTFAID – “A knowledge based platform of services for supporting medical-clinical management of heart failure within elderly population”, which is scheduled to start early in 2006. D. Gamberger will lead research activities under WP4 (work-package 4): “Knowledge representation, discovery and management”



Logo of the HEARTFAID project

Technological projects and activities

“Quantum Random Bit Generator”, (B. Medved Rogina, project leader Mario Stipčević) World Bank project “Quantum Random Bit Generator for applications in cryptography, Monte Carlo simulations and research” (funded by the World Bank, Technology Assistance program TAL-2, 2004-2005, project leader Mario Stipčević, Division of Experimental Physics) which resulted in construction of one fast non-deterministic random number generator with bit rate of 12Mb/s. Invention and prototype “Quantum random number generator” was awarded by two international gold medals and the award for innovations in 2005);

CRO-GRID, - technology project financed by Croatian Ministry of Science, Education and Sport - collaboration on development of grid applications;

Laboratory for stochastic signals and processes collaborates with Faculty of Kinesiology and with School of Dental Medicine from University of Zagreb on development of measurement methodology and data acquisition protocols for human locomotion and human jaw kinematics analysis.

EDUCATIONAL ACTIVITIES

1. Knowledge Discovery in Medical Domains, Dragan Gamberger, PhD Program at the Medical School, University of Zagreb.
2. Optical communication networks, Lectures (B. Medved Rogina), Faculty of Electrical Engineering and Computing, (FER) Zagreb,
3. Police operational techniques, Lectures (B. Medved Rogina), Police Academy, Zagreb,
4. Algorithms in Bioinformatics, Lectures (S. Ristov), postgraduate study, Faculty of Electrical Engineering and Computing, (FER) Zagreb

SELECTED PUBLICATIONS

1. Gamberger D, Krstačić A, Krstačić G, Lavrač N, Sebač, M. Data analysis based on subgroup discovery: Experiments in brain ischemia domain. Proceedings of IDAMAP 2005 Workshop at 10th European Conference on Artificial Intelligence in Medicine (AIME-05) 2005:52.
2. Topić G, Šmuc T, Šojat Z, Skala K. Reimplementation of the Random Forest Algorithm, Proceedings of Parallel Numerics, Theory and Applications, Vajtersic M. et al. (ed.). Salzburg, 2005: 119.
3. Ristov S. LZ trie and dictionary compression, Software: Practice & Experience. 2005: 35: 445.
4. Supek F, Šmuc T, Lučić B. A prototype structure-activity relationship model based on National Cancer Institute cell line screening data. Period Biol 2005:107: 451.
5. Marić I, Galović A, Šmuc T. Calculation of Natural Gas Isentropic Exponent. Flow Measur Instrum 2005: 16: 13.
6. Vojnović B, Medved Rogina B. Optimum Processing for Precise Ultra-Wide-Band Pulse Carrier-Signal Timing, Proceedings of the 28th International Convention MIPRO'05, Opatija, 2005: 153.
7. Medved Rogina B, Michieli I. Metastability parameters evaluation by DSO data acquisition. Proceedings of the International Conference IWSSIP 2005, 12th International Workshop on Systems, Signals & Image Processing, Greece, 2005: 397.

Division of Physical Chemistry



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

DIVISIONAL ORGANISATION

Head: Aleksandar Sabljic

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

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

OVERVIEW OF THE DIVISION

In 2005, members of the Division published 55 contributions in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical chemistry, modelling of physical and chemical processes, structural and chemical analyses, and in biosciences. A significant part of these works was published

in the highest ranking journals in chemistry, such as Chemistry-A European Journal, Inorganic Chemistry, the Journal of Physical Chemistry, and the Journal of the American Society for Mass Spectrometry. Division members contribute extensively (36 courses) to undergraduate and graduate education and have organized highly regarded scientific conferences. All this is achieved within the framework of traditional international collaboration with Harvard University, Rice University, Pacific Northwest Laboratory, Free University Berlin, Hebrew University of Jerusalem, to mention but a few.

TOP ACHIVEMENTS

Novel cyclopalladated complexes

Palladocycles are one of the most popular and investigated classes of cyclometalated compounds due to their extensive application in organic synthesis, catalysis, photochemistry and in the design of new metallomesogenes. We have prepared the first examples of doubly cyclopalladated azobenzenes and structures were determined by X-ray analysis and NMR spectroscopy. Quantum-chemical calculations indicated that these structures are indeed the

most stable among all isomers conceivable by varying the solvent heteroatoms coordinated to the palladium atom and relative positions of solvent molecules and chlorine atom. (M. Ćurić et al., *Inorg Chem* 2005: 44: 5975). Two metalated phenyl rings and two easily replaceable solvent ligands make these complexes excellent building blocks for designing a wide variety of metallomesogenes, organometallic polymers and even more elaborate supramolecular systems.

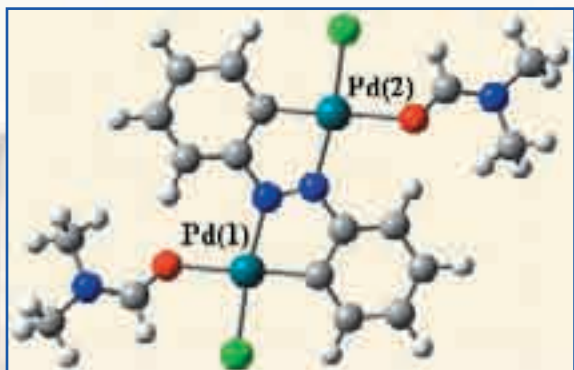


Figure 1: Dipalladated azobenzene complex, $\{PdCl(dmf)\}_2(\mu-C_6H_4N=NC_6H_4)$

Irradiative degradation of L-alanine

The two-dimensional hyperfine sub-level correlation (2D-HYSCORE) spectra of the L-alanine γ -irradiated crystal were measured to detect possible contribution of ^{14}N hyperfine splitting to the spectrum of stable radical centres. The ^{14}N hyperfine and quadrupole tensors are evaluated and assigned to abstracted NH_3 molecule, which is a product of the first stable radical formation. The obtained results can be used as potential new elements

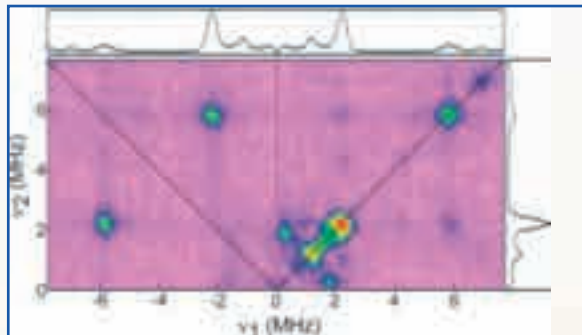


Figure 2: 2D-HYSCORE spectra of the γ -irradiated L-alanine

for description of the environment of the first stable L-alanine radical in the crystal lattice (B. Rakvin and N. Maltar-Strmečki, *Chem Phys Lett* 2005: 415: 161).

Control of surfactants self-assembly

The self-assembly process of amphiphilic molecules in water results in the formation of a wide range of supramolecules. To design micelles, vesicles and tubules of optimal performance for specific application two approaches have been used: (i) synthesis of new surfactants by altering their structural elements and (ii) modification of conditions in aqueous solution. The second approach enables formation of giant vesicles and tubules at proper molar ratio of the cationic surfactant and oppositely charged biopolymers or oppositely

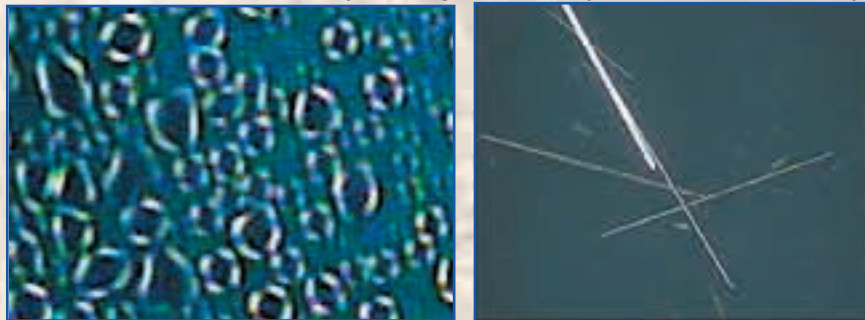


Figure 3: Representative polarization microphotographs of (a) giant vesicles from surfactants/biopolymer mixtures and (b) tubules from gemini surfactant/bile salt mixtures

charged surfactants in catanionic mixtures (V. Tomašić et al., J Colloid Interf Sci 2005: 285: 342). Investigated structures are promising novel systems for drug and gene delivery, cosmetic formulations, templates for microscale metal tubules for electronic and magnetic materials, etc.

Proton transfer in macrocycles

The chemistry of mixed-donor macrocycles has attracted continuous attention due to their ability to bind selectively different chemical species. Diffusion of proton in the dioxo-diaza heteromacrocyclic compound was investigated by crystallographic and spectroscopic studies. Transfer of proton either inside or outside the macrocyclic cavity imposes different hydrogen bond networks which stabilize the binding site of the proton in the protonated macrocyclic species (Lj. Tušek-Božić, Polyhedron 2005: 24: 97).

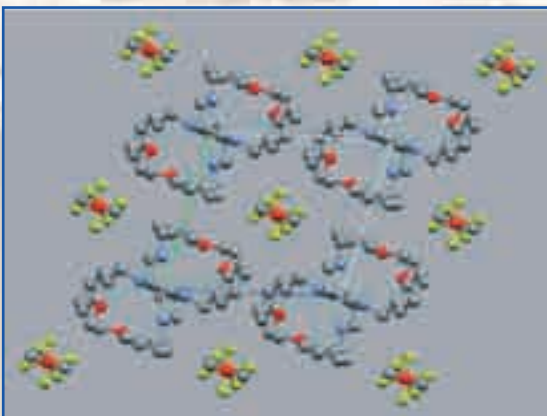


Figure 4: The crystal packing of $[H(L)_2]PF_6$ ($L=5,6,14,15$ -dibenzo-1,4-dioxo-8,12-diazacyclopentadeca-5,14-diene)

Structural analysis of hydrolases with a novel $\alpha/\beta/\alpha$ fold

A large family of hydrolases (770 proteins sequences) with low sequence similarity revealed four conserved blocks including characteristic amino acids SGNH in each of them. However, for only 10 of those proteins sequences the 3D structures are known. Bioinformatics was used to characterize them (B. Kojić-Prodić et al., Acta Cryst A 2005: 61: C42). The analysis shows a new characteristic $\alpha/\beta/\alpha$ fold with a well preserved topology of the catalytic site. The striking fact is that among these hydrolases, multifunctional enzymes were recognized. Our novel lipase from *Streptomyces rimosus* also belongs to this family.

EDUCATIONAL ACTIVITIES

Division provides annually nearly 40 undergraduate and graduate courses at Universities in Zagreb, Split, Rijeka and Osijek.

AWARDS

Marko Rožman, Annual award for young scientist of The Society of University Teachers and Scientists

SELECTED COLLABORATIONS

1. Investigations of calcium phosphate based biomaterials, FP6 Specific Support Action - Creating international cooperation teams of excellence in the field of emerging biomaterial surface research, Maja Dutour Sikirić

2. Origin of Life and Early Evolution, Vesna Noethig-Laslo (COST chemistry D-27 action)
3. Protein-Lipid Interactions, Greta Pifat-Mrzljak (COST chemistry D-22 action)
4. Advanced Paramagnetic Resonance Methods in Molecular Biophysics, Boris Rakvin (COST physics P-15 action)

SELECTED INVITED LECTURES

1. L. Klasinc, Atmospheric transport of pollutants from urban areas, 40th IUPAC Congress-Innovation in Chemistry, Beijing, 14-19 August 2005.
2. I. Habuš, Diels-Alder reactions on imines derived from 3-amino- β -lactams, Stony Brook Symposium on New Horizons in Organic Chemistry: Stony Brook Alumni Symposium, State University of New York at Stony Brook, NY, USA, 2005.
3. B. Kojić-Prodić, Bioinformatics approach to characterisation of SGNH hydrolases, XX Congress of the International Union of Crystallography, Florence, Italy, 26 August 2005.
4. T.P. Živković, Einstein: In a search of quantum meaning – from the EPR paper (1935) through Bells inequalities (1964) to the Aspect experiment (1980), 20th MATH/CHEM/COMP, Dubrovnik, 20-25 June 2005.
5. N. Došlić, Hydrogen-bonded prototype systems: A computational approach to spectroscopy, Graduiertenkolleg "Hydrogen Bonding and Hydrogen Transfer", Frei Universität Berlin, Berlin, Germany, 29 June 2005.

CONFERENCES ORGANIZED BY SCIENTISTS OF THE DIVISION

1. 20th MATH/CHEM/COMP, Dubrovnik, 20-25 June 2005
2. 1st South-Eastern European Workshop on Practical Approaches to Computational Biology, Opatija, 1-4 September 2005
3. Workshop: Preparation and properties of functionalized vesicles as protocell models, COST D 27 Action: Origin of Life and Early Evolution, Zagreb, 20-21 May 2005

PROJECTS

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

1. Properties and behaviour of atmospheric microconstituents, Tomislav Cvitaš
2. Surfactants, processes in solution and at interfaces, Nada Filipović-Vinceković
3. Reactivity and reaction mechanism, Leo Klasinc
4. Investigation on chemical reactivity and ultrafast processes, Aleksandar Sablić
5. Development and application of models in chemistry and bioinformatics, Nenad Trinajstić
6. Structural and biological investigation of new complex compounds, Ljerka Tušek-Božić
7. Structure and dynamics of (bio)molecules, Biserka Kojić-Prodić
8. Biophysics of lipoprotein interactions with active substances, Greta Pifat-Mrzljak
9. Electron spin resonance in systems with paramagnetic particles, Boris Rakvin

10. Modelling of novel carbon materials, Ante Graovac
11. Interactions of biomembranes with amino acids and peptides, Vesna Nöthig-Laslo
12. Multidisciplinary sedimentological investigations, Halka Bilinski
13. Matter under extreme conditions, Slobodan Bosanac
14. Description and behavior of quantum systems in interaction, Tomislav Živković
15. Custom DNA synthesis, Ivan Habuš

Other projects

1. Combined quantum mechanical and force field approaches in study of molecules of biological and biotechnical interest, S. Tomić (Bilateral project with Austria)
2. Functional organisation of noncovalent complexes of bacterial lipases, B. Kojić-Prodić (Bilateral project with Austria)
3. Structure and dynamics of biomolecules, M. Luić (Bilateral project with Slovenia)
4. Interactions of liposomes with aminoacids and peptides for targeted incorporation into organism studied by Electron Spin Resonance, V. Noethig-Laslo (Bilateral project with Slovenia)
5. Cell membranes and oxidative stress, G. Pifat-Mrzljak (Bilateral project with Slovenia)
6. Synthesis of organometallic compounds in mass spectrometer, D. Srzić, (Bilateral project with Slovenia)
7. Investigation of structure and dynamics of proteins with numerical methods, S. Tomić, (Bilateral project with Slovenia)
8. Microbial lipases - search for new biocatalysts, A. Višnjevac (Bilateral project

with Slovenia)

9. Electronic structure of halogenated diphenylmethanones and diphenylethanones, B. Kovač (Bilateral project with Slovenia)
10. Cyclopalladated complexes of azobenzenes, M. Ćurić (Bilateral project with Slovenia)
11. Formation, transport and degradation of photooxidants in the Mediterranean area, N. Kezele (Bilateral project with Slovenia)
12. Research of new materials based on carbon, A. Graovac (Bilateral project with Slovenia)

SELECTED PUBLICATIONS

1. Bosanac SD: Dynamics of particles and the electromagnetic field, World Scientific, Singapore, 2005: pp 496.
2. Ćurić M, Babić D, Višnjevac A, Molčanov K: Simple route to the doubly ortho-palladated azobenzenes: Building blocks for organometallic polymers and metallomesogenes. *Inorg Chem* 2005: 44: 5975.
3. Škorić I, Basarić N, Marinić Ž, Višnjevac A, Kojić-Prodić B, Šindler-Kulyk M: Synthesis and photochemistry of β,β' -di(2-furyl) substituted o-divinylbenzenes. Intra- and/or intermolecular cycloaddition as an effect of annelation. *Chemistry-A Eur J* 2005: 11: 543.
4. Ljubić I, Sabljic A: Ozonolysis of fluoroethene. Theoretical study of unimolecular decomposition paths of primary and secondary fluorozone. *J Phys Chem A* 2005: 109: 2381.
5. Novak I, Kovač B: Halogens in com-

- petition: Electronic structure of mixed dihalobenzenes. *J Phys Chem A* 2005: 109: 3318.
6. Ljubić I, Sabljic A: Dibenzo-p-dioxin. An ab initio CASSCF/CASPT2 study of the π - π^* and n - π^* valence excited states. *J Phys Chem A* 2005: 109: 8209.
7. Rožman M: The gas-phase H/D exchange mechanism of protonated amino acids. *J Am Soc Mass Spectr* 2005: 16: 1846.
8. Vukičević D, Grubeša T, Graovac A: An efficient method to enumerate topologically distinct clusters of hydrogen-bonding in water molecules. *Chem Phys Lett* 2005: 416: 212.
9. Cvitaš T, Klasinc L, Kezele N, McGlynn SP, Pryor WA: New directions: How dangerous is ozone? *Atmos Environ* 2005: 39: 4607.
10. Sikirić M, Primožič I, Talmon Y, Filipović-Vinceković N: Effect of the spacer length on the association and adsorption behavior of dissymmetric gemini surfactants. *J Colloid Interf Sci* 2005: 281: 473.

Division of Organic Chemistry and Biochemistry



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

ZOKB

DIVISIONAL ORGANISATION

Head: Kata Majerski (acting head until 10.06.2005), Mirjana Eckert-Maksić (from 10.06.2005)

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

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

OVERVIEW OF THE DIVISION

Research activities in the Division of Organic Chemistry and Biochemistry during 2005 encompassed a wide spectrum of topics including modern organic syntheses, physical organic and supramolecular chemistry, spectroscopic and quantum mechanical studies of organic systems, and experimental and theoretical investigations of biologically important peptides, glycopeptides and proteins. It should be emphasized that this research is multifaceted, since it covers aspects of materials science as well as environmental and medicinal chemistry. Another characteristic feature of the work is a good blend of fundamental and applied research. The main body of the results was published in 44 scientific papers, which appeared mostly in renowned scientific journals. Concerning the applicable aspects of the research, it is noteworthy that new approaches have been developed in the synthesis of novel compounds potentially useful in anticancer chemo- and photodynamic therapy. Furthermore, a new class of the environmentally friendly organocatalysts has been designed and prepared. Last but not least, the first spin-off company of the Institute "Biozyne" was started.

The Division fosters intramural and extramural collaboration including Universities in Zagreb and Osijek, and a number of research centres abroad, as evidenced by a significant number of joint papers. Members of Division have made significant contributions to higher education by providing 9 courses at undergraduate and postgraduate levels and by supervising a number of B.Sc. (7), M.Sc. (1) and Ph.D. (3) thesis. They are also active in a number of national and international societies (bodies) and serve in journal editorial boards, as well as referees for leading scientific journals.

TOP ACHIEVEMENTS

New achievements in organic synthesis

A facile and efficient one-pot synthesis of a variety of alicyclic and aliphatic nitriles by treatment of carboxylic acids with MeCN and sulfuric acid has been reported (K. Mlinarić-Majerski et al., *Synlett* 2005: 13: 2089). Highly efficient high-pressure synthesis of new rod-like and U-shaped polycyclic compounds containing two 7-sila- or 7-germanorbornene units fused to 7-oxanorbornene rings is reported. These are the first examples of homonuclear bis-metallated polycyclic compounds reported in literature (M. Eckert-Maksić et al., *Eur J Org Chem* 2005:21:4612). Synthesis of a novel type of guanidine superbases involving multiple intramolecular hydrogen bonding has been also described (Z. Glasovac et al., *Tetr Lett* 2005: 46: 8733).

A series of new N-sulfonylpyrimidines (M. Pavlak et al., *Cancer Res Clin Onc* 2005:

131: 829), as well as a variety of new peptides containing different unnatural adamantane amino acids were synthesized and tested against several tumour lines. Some of these compounds showed anticancer activities (Š. Horvat et al., Patent Appl. P 20050242A, PCT/HR05/0031). The synthesis of new photoinduced gelation systems starting from stilbene-containing oxalamide gelators was also reported (S. Miljanić et al., *Langmuir* 2005: 21: 2754).

Finally, the synthesis and analysis of the separation efficacy of six new chiral packing materials for high performance liquid chromatography, consisting of 4- or 2-chloro-3,5-dinitrobenzoic acid, L-alanine and different π -donor units, was published (I. Gazić et al., *Tetrahedron: Asymmetry* 2005: 16: 1175).

Computational design of superacids and superbases

It was shown that a combination of Schwesinger's phosphazene concept and Alder's idea of a disubstituted 1,8-naphthalene spacer provided a new superbase HMPN, which represents the most basic "proton sponge" synthesized so far for this type of compounds (V. Raab et al., *J Am Chem Soc* 2005: 127: 15738). Further, an efficient strategy in tailoring neutral organic superacids of unprecedented strength has been developed. It includes a selection of suitable molecular skeletons and their careful dressing by CN groups. In this way powerful superacids are obtained, which surpassed the acidity of sulfuric acid by 40-50 orders of magnitude (R. Vianello and Z. B. Maksić, *Chem Commun* 2005: 3412).

Calculation of optical-rotatory dispersion

In collaboration with research groups of K. Nakanishi (Columbia University, New York, USA) and C. Rosini (University Basilicata, Potenza, Italy), members of the research group of Z. Hameršak reported ab initio calculations of optical rotations (OR). It was demonstrated that ab initio calculations of ORD curves provide a reliable method for the assignment of absolute configuration of these conformationally flexible molecules (E. Giorgio et al., J Org Chem 2005: 70: 6557). The illustration describing this work (Figure 1) was chosen to appear on the front cover of volume 70, number 17 of the Journal of Organic Chemistry as well as on the front cover of the 2006 wall calendar produced by the same journal.



Figure 1: The front cover of volume 70, number 17 of the Journal of Organic Chemistry. The illustration pertains to research detailed in E Giorgio et al., J Org Chem 2005: 70: 6557.

Understanding the suicide inactivation of EAL

Ethanolamine ammonia lyase (EAL) is a coenzyme B₁₂-dependent enzyme that catalyzes the deamination of amino alcohols. Certain analogues of the natural substrate have, however, been found to inactivate the enzyme after initial binding. By studying the mechanism of these reactions with ab initio molecular orbital calculations, it was found that the most common driving force of the suicide inactivation was the formation of a radical intermediate that is too stable to undergo further reaction (G. Sandala et al., J Am Chem Soc 2005: 127: 8856)

New approach to photodynamic therapy

In collaboration with the research group of G. Karminski-Zamola from the Faculty of Chemical Engineering and Technology a photo-induced switching of DNA inactive substances into DNA intercalators was discovered. The method enables a new approach to photodynamic therapy (S. Starčević et al., J Am Chem Soc 2005: 127: 1074; I. Jarak et al., J Med Chem 2005: 48: 2346).

Towards understanding a mechanism of tissue damage in diabetes

Humoral MG level in patients with diabetes having good and poor disease control was analysed using HPLC assay, based on methylglyoxal derivatization. The study indicated that an increased production of toxic aldehydes may be a part of mechanisms that promote tissue damage in diabetes (I. Nemet et al., Clin Biochem 2005: 38: 379).

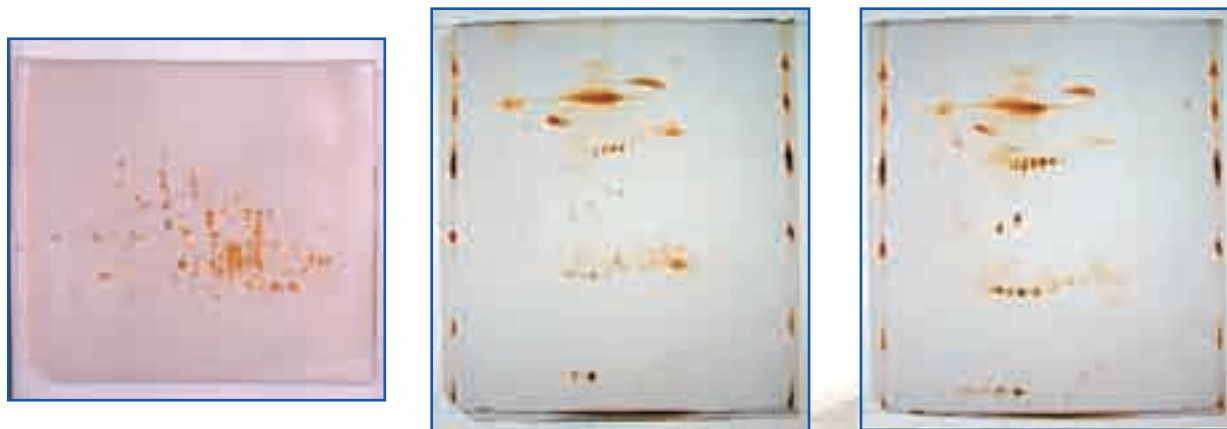


Figure 2: Two dimensional electrophoresis (2-DE) gel images of a bacterial lysate of *E. coli* BL21 (A) and of cerebrospinal fluid proteins (B) of patients suffering of non-inflammatory neurological disorders (left) and multiple sclerosis (right); 2-DE was performed by isoelectric focusing in non-linear pH gradient 3 – 10 as the 1st dimension, followed by electrophoresis in a 12% homogeneous polyacrylamide gel under denaturing conditions as the 2nd dimension. Protein spots were visualized by silver staining.

On the way to finding new disease markers

The control of overexpression of human dipeptidyl peptidase III in bacteria *E. coli* has been performed by using a new high-resolution two-dimensional gel electrophoresis technique. The method was also applied in order to check protein homogeneity of several purified enzymes and to search for differentially expressed proteins in cerebrospinal fluids obtained from patients suffering neurological disorders. The latter exercise is expected to lead to new disease markers (Figure 2).

Žinić

5. Design and Synthesis of Bioactive Peptides, Glycopeptides and Biomarkers, Štefica Horvat
6. Reactive Intermediates in Ground and Excited State, Mirjana Eckert-Maksić
7. Hydrolases – from Isolation to Function, Marija Abramić
8. Extended π -Systems and Molecular Spectroscopies, Goran Baranović
9. Proton Affinity and Proton Transfer Reactions in Chemistry, Zvonimir Maksić
10. Germanium, Silicon and Tin Contained Polycyclic Structures, Davor Margetić
11. Computational Studies of Protein Structure and Function (from April 22nd), David Smith

International and collaborative projects

1. Photoinduced Proton Transfer in Biologically Active Molecules – Theoretical Investigation, Bilateral Croatian-Austria project, M. Eckert-Maksić
2. Lipide crystals of bent-core mesogens, Bilateral collaboration with UK (till August 31), A. Lesac
3. Simulation of Proton Dynamics in Systems of Biological Interest, Bilateral Croatia-Slovenia project, Z. Maksić
4. Thermally Processed Foods: Possible Health Implication, COST Action, working group

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

1. Stereoselective Synthesis and Catalysis, Zdenko Hameršak
2. New Optically Active Materials, Vladimir Vinković
3. Synthesis, Molecular Structure and Function of Polycyclic Molecules, Kata Majerski
4. Supramolecular Organization of Gels, Molecular Recognition and Catalysis, Mladen

D927, Š. Horvat

5. Intrinsic Reactivity of New Materials COST Action, working group D26/0014/03, M. Eckert-Maksić
6. Intrinsic Reactivity of New Materials COST Action, working group D26/0014/03, Z. Maksić
7. Transcription of Bioinspired and Designed Functional Modules into Nanostructured Smart Gels, COST Action, working group D31, M. Žinić

Research and development projects

1. Design and Synthesis of Steroids and Steroid-like Derivatives (TECNA s.r.l. Area di Ricerca, Padriciano, Trieste, Italy), K. Majerski
2. Modelling and Simulation of Protein Folding and the Catalytic Role of Enzymes, (subproject under CRO-GRID MZOŠ-HITRA project), Z. B. Maksić

AWARDS

Award to Kata Majerski: Croatian state annual award for science in the field of natural sciences.

Award to Mirjana Eckert-Maksić: Annual award of the City of Zagreb for scientific achievements in physical-organic chemistry.

Awards to Nikola Basarić: Croatian state annual award for young scientists in the field of natural sciences, as well as the "Vladimir Prelog" award for young scientists of Croatian Chemical Society and PLIVA d.d. and award for young scientists from The Society of University Teachers and Scientists, Zagreb.

Award to Borislav Kovačević: Leopold Ružička award for young scientists of the Croatian Chemical Society.

SELECTED INVITED TALKS

1. Smith D.: The Substrate Mechanism of Pyruvate Formate-Lyase: The Influence of the Environment on Enzyme-Catalyzed Reactions Involving Free Radicals, WATOC

2005, 7th Congress of the World Association of Theoretically Oriented Chemists. Cape Town, South Africa, 16.-21. 1. 2005.

2. Smith D.: Investigation of the Structure and Function of Biologically Important Molecules: What Can Computers Tell Us?, DFG-Priority Programme Workshop: Radical in Enzymatic Catalysis. Schloss Rauischholzhausen, Germany, 11.-13. 4. 2005.
3. Kovačević B.: Computational Design of Neutral Organic Superbases in the Gas Phase and in Acetonitrile. XIX Croatian Meeting of Chemists and Chemical Engineers. Opatija, Croatia, 24.-27. 4. 2005.
4. Basarić N.: Pyrrole compounds in the excited state, useful synthetic tools and analytical reagents. XIX Croatian Meeting of Chemists and Chemical Engineers. Opatija, Croatia, 24.-27. 4. 2005.
5. Smith D.: The Integrated Molecular Orbital Approach to Accurate Calculations of Large Molecular Systems. 1st South Eastern European Workshop on Practical Approaches to Computational Biology. Opatija, Croatia, 1.-4. 9. 2005.
6. Žinić M.: Supramolecular Chemistry and Stereochemistry of Gel Assemblies. ESF Research Conference Supramolecular Chemistry. Molecular Architectures and Systems. Obernai, Strasbourg, France, 14.-19. 10. 2005.
7. Smith D.: Theoretical Study of the Mechanism of Pyruvate Formate-Lyase. Pacificchem, 2005 International Chemical Congress of Pacific Basin Chemical Societies. Honolulu, Hawaii, USA, 15.-20. 12. 2005.

PATENT APPLICATIONS

1. Horvat Š., Majerski K., Glavaš-Obrovac Lj., Jakas A., Veljković J., Roščić M., Kragol G., Karner I., Synthetic peptides containing unnatural adamantane-related amino acids for use as antitumor drugs (P 20050242A, PCT/HR05/0031)
2. Maksić M., Glasovac Z., "N,N',N"-Tris-(3-

dimethylaminopropyl)guanidine. The procedure of preparation from carbodimide and application in reactions of oil", (P20040341 A, 3125.07.2005; PCT/HR2005/000026).

PUBLICATIONS

1. Starčević K, Karminski-Zamola G, Piantanida I, Žinić M, Šuman L, Kralj M. Photoinduced switch of a DNA/RNA inactive molecule into a classical intercalator. *J Am Chem Soc* 2005: 127: 1074.
2. Raab V, Gauchenova E, Merkoulou A, Harms K, Sundermeyer J, Kovačević B, Maksić Z. 1, 8-Bis(hexamethyl-triamino-phosphazeny) naphthalene, HMPN: A superbasic bisphosphazene "Proton Sponge". *J Am Chem Soc* 2005: 127: 15738.
3. Sandala, GM, Smith DM, Radom L. Divergent mechanisms of suicide inactivation for ethanolamine ammonia-lyase. *J Am Chem Soc* 2005: 127: 8856.
4. Vianello R, Maksić Z. Extremal acidity of Rees polycyanated hydrocarbons in the gas phase and DMSO - a density functional study. *Chem Commun* 2005: 27: 3412.
5. Jarak I, Kralj M, Šuman L, Pavlović G, Dogan J, Piantanida I, Žinić M, Pavelić K, Karminski-Zamola G. Novel cyano- and N-isopropylamidino-substituted derivatives of benzo[b]thiophene- 2-carboxanilides and benzo[b]thieno[2, 3-c]quinolones: Synthesis, photochemical synthesis, crystal structure determination and antitumor evaluation. Part 2. *J Med Chem* 2005: 48: 2346.
6. Giorgio E, Roje M, Tanaka K, Hameršak Z, Šunjić V, Nakanishi K, Rosini C, Berova Nina. Determination of the absolute configuration of flexible molecules by ab initio ORD calculations: a case study with cytotoxazones and isocytotoxazones. *J Org Chem* 2005: 70: 6557.
7. Mlinarić-Majerski K, Margeta R, Veljković J.

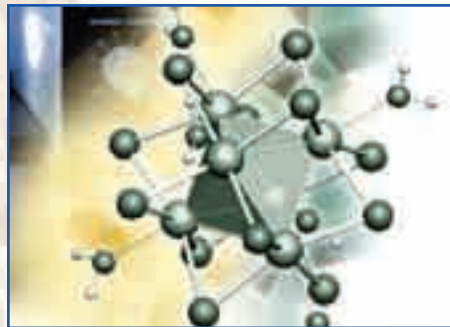
A facile and efficient one-pot synthesis of nitriles from carboxylic acids. *Synlett* 2005: 2089.

8. Eckert-Maksić M, Margetić D, Kirin S, Milić D, Matković-Čalogović D. Synthesis of fused norbornenes containing two 7-metallonorbornene units assisted by high pressure. *Eur J Org Chem* 2005: 21: 4612.
9. Gazić I, Kontrec D, Lesac A, Vinković V. The enantiomeric recognition of dihydropyrimidonic compounds by chiral selectors derived from 4- or 2-chloro-3, 5-dinitrobenzoic acid. *Tetrahedron: Asymmetry* 2005: 16: 1175.

Book Chapters

1. Eckert-Maksić M, Maksić Z. Antiaromaticity and aromaticity in carbocyclic four-membered rings. In: *The Chemistry of Cyclobutanes*, Rappoport Z, Liebman JF. (editors); Chichester: John Wiley, 2005.
2. Fages F, Vogtle F, Žinić M. Systematic design of amide- and urea-type gelators with tailored properties. In: *Low molecular mass gelators: design, self-assembly, function*, Topics in current chemistry, Fages F. (editor). Berlin: Springer-Verlag, 2005.
3. Žinić M, Vogtle F, Fage F. Cholesterol-based gelators. In: *Low molecular mass gelators: design, self-assembly, function*, Topics in current chemistry. Fages, F. (editor). Berlin: Springer-Verlag, 2005.
4. Warrenner RN, Margetić D, Mann DA, Chen Z-L, Butler DN. Novel geometry polynorbornane scaffolds for chromophore linkage and spacing. In: *Artificial Photosynthesis: From Basic Biology to Industrial Application*, Collings AF, Critchley C. (editors). Weinheim: Wiley-VCH, 2005.

Division of Materials Chemistry



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

DIVISIONAL ORGANISATION

Head: Svetozar Musić

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

- ⇒ Laboratory for synthesis of new materials, Boris Subotić
- ⇒ Laboratory for precipitation processes, 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, Rozelinda Čož-Rakovac

and inorganic biomaterials. An important research activity is the study of the kinetics and mechanisms of various processes in solid/liquid heterogeneous systems. Members of the group for ichtiopathology-biological materials have been very active in the formation of the Centre for diagnostics of Fish, Shellfish and Crustaceans Diseases. The radiation chemistry and dosimetry laboratory at the division is the only existing unit in Croatia which has been dealing with all aspects of the physico-chemical effects of ionizing radiations. We possess a strong cobalt-60 source for commercial irradiations. The low-dose and high dose chemical dosimetry systems were developed and internationally accepted. The secondary standard dosimetry laboratory was established. The Division also participated in numerous cooperative activities with different industries, hospitals, state institutions and the University of Zagreb

OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is strongly focused on the synthesis of new functional materials and investigation of their chemical, microstructural and physical properties. We are investigating magnetic and nonmagnetic metal oxides, glass-ceramics, cluster compounds, organic polymers, intermetallic compounds, metal hydrides

TOP ACHIEVEMENTS

Mechanism and kinetics of zeolite crystal growth

The crystal growth of zeolites was found to be independent of size and governed by the reaction of monomeric and/or low-molecular aluminate, silicate and aluminosilicate anions from the liquid phase on the surfaces of growing zeolite crystals. In

contrast to strong influence of the ratio Si/Al in the liquid phase on the growth rate, and even type of zeolite formed, the crystal size distribution of the crystalline end product (pure zeolite A, mixtures of zeolites A and X, pure zeolite X) is independent on the chemical composition of the liquid phase, which represents additional evidence for the gel “memory” effect (S. Bosnar et al., Croat Chem Acta 2005: 78: 1).

Solid solutions in $\text{HfO}_2\text{-Al}_2\text{O}_3$ and $\text{ZrO}_2\text{-Al}_2\text{O}_3$ systems

The crystallization temperature of the amorphous precursors of the $\text{HfO}_2\text{-AlO}_{1.5}$ and $\text{ZrO}_2\text{-AlO}_{1.5}$ systems was found to increase with increasing $\text{AlO}_{1.5}$ content, from 530 °C (0 mol % $\text{AlO}_{1.5}$) to 940 °C (60 mol % $\text{AlO}_{1.5}$) and from 405 °C (0 mol % $\text{AlO}_{1.5}$) to 915 °C (60 mol % $\text{AlO}_{1.5}$). Crystallization products with $\text{AlO}_{1.5}$ -contents ≤ 50 mol % were only obtained in the presence of HfO_2 - and ZrO_2 -type solid solutions. The lattice parameters of the ZrO_2 -type solid solutions decreased with increasing Al^{3+} content up to ~ 10 mol %, whereas above 10 mol %, further increases of the Al^{3+} content had a very small influence on the unit-cell volume

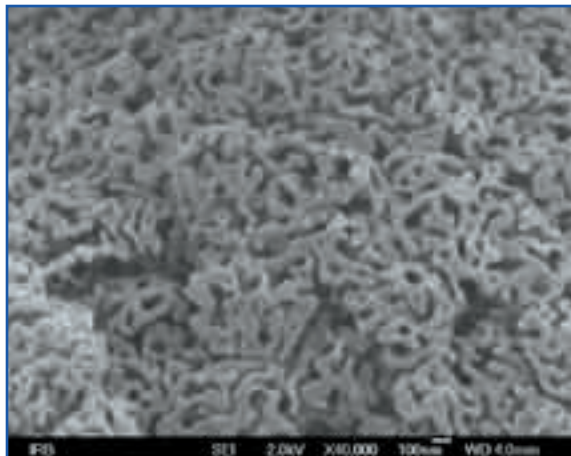


Figure 2: Microporous hematite ($\alpha\text{-Fe}_2\text{O}_3$) synthesized in our division

of both HfO_2 - and ZrO_2 -type solid solutions. The solubility of Hf^{4+} , and Zr^{4+} ions in the aluminium oxides lattice appeared to be negligible. (G. Štefanić et al., J Alloys Comp 2005: 388: 126).

Multifunctional PC Controlled Bench Scale Chemical Reactor (VIKER)

In the framework of a HITRA project, a multi-purpose PC-controlled bench-scale chemical reactor (VIKER) has been constructed and PID regulation implemented. The reactor has the possibility to control a number of technological parameters. Its



Figure 1: High resolution scanning electron microscope



Figure 3: Home-made multi-purpose PC controlled chemical reactor VIKER

adaptability is achieved by the incorporation of different actuators and sensors, which enable conducting the process using solid, liquid or gas reactants. The chemical process is controlled by home-made electronics, software and intuitive graphical interface. (J. Kontrec et al., Coll Antropol 2005: 29: 289).

Dosimetry

An ethanol – chlorobenzene dosimetry system for high dose measurements was prepared for the forthcoming ICRU Report. A new draft of the Standard Practice for Use of an Ethanol–Chlorobenzene Dosimetry System (ISO/ASTM Standard 51538) underwent major revision and has been accepted by the ASTM (American Society for Testing and Materials) Subcommittee E10.01 in 2005. Based on the received comments a revised draft was prepared for balloting as a Final Draft International Standard (FDIS) by the ISO/ASTM Committee in 2006. Once approved, the international standard will be in force for the next 5 years. (D. Ražem. In: IAEA Trends in Radiation Sterilization. IAEA Report Vienna 2005: 135).



Figure 4: Work with radiophotoluminescence dosimetry reader

Compatibilization of polypropylene/talc composites

The study of the structure-property relationships of compatibilized isotactic polypropylene (iPP)/talc composites is important for the property optimization of superior plastics for the automotive industry. The encapsulation extent of talc crystals (core-shell effect) and some mechanical properties as a measure for the compatibilization effect of (iPP)/talc composites with different styrene rubber block copolymers (SRBC)(SBS, SEP, SEBS, and SEBS-g-MA) seemed to decrease along the series SEBS-g-MA > SEBS > SBS > SEP, affected by different factors. The significantly higher impact strength observed for iPP/talc/SEBS composites than for other (iPP)/talc/SRBC composites and iPP/SRBC blends indicates a superimposing effect of additional influencing factors (M. Denac et al. Composites A 2005: 36: 1094; M. Denac et al. Composites A 2005: 36: 1282).

New hydrogen storage materials

New rare earth based intermetallic compounds of the composition $\text{RENi}_{3.5}\text{Al}_{1.5}$ (RE = Y, Tb, Dy, and Ho) compounds were prepared and charged with hydrogen. It was found that under 1.5 MPa gas pressure, the maximum hydrogen capacity varies with the rare earth atom from 3.8, 2.8, 3.9 to 2.42 H atoms / alloy formula unit for Tb, Dy, Ho and Y, respectively. Neutron diffraction studies indicated that hydrogen (deuterium) atoms occupy only two of the five possible sites in the crystal structure. Magnetisation measurements of $\text{TbNi}_{3.5}\text{Al}_{1.5}$ show strong ferromagnetic contribution supported by magnetic terbium, while the exchange couplings with nickel remain rather weak. The

TbNi_{3.5}Al_{1.5} - hydride reveals a reinforcement of the magnetic couplings, indicating that nickel is magnetically polarised but in an opposite manner to terbium. (B. Šorgić et al. J Alloys Compd 2005: 404-406: 64).

New clusters of Nb and Ta

The solutions of hexanuclear halide clusters of niobium and tantalum in aliphatic nitriles could be suitable media for the preparation of cluster compounds containing two or more differently charged cluster entities in the same formula unit. Thus, by partial oxidation of a solution of tantalum chloride clusters in n-butyl cyanide (n-C₄H₉CN, n-BuCN) the double salt of composition 2[(Ta₆Cl₁₂)Cl₃(n-BuCN)₃]·[(Ta₆Cl₁₂)Cl₄(n-BuCN)₂]·n-BuCN has been prepared. The coexistence of differently charged cluster units, namely [Ta₆Cl₁₂]³⁺ and [Ta₆Cl₁₂]⁴⁺ in [(Ta₆Cl₁₂)Cl₃(n-BuCN)₃] and [(Ta₆Cl₁₂)Cl₄(n-BuCN)₂], respectively, makes this species unique in the transition-metal cluster chemistry. The compounds of this type could be interesting from the point of view of the intercluster transfer of charge. Also, this is the first structurally characterized complex compound with coordinated n-BuCN (P. Planinić et al. Comptes Rendus Chimie 2005: 8: 1766).

Structural properties of conducting oxide Sb-doped SnO₂ (ATO)

Antimony-doped tin oxide (ATO) samples with doping level up to 14 at% Sb were hydrothermally prepared and characterized by X-ray diffraction and ¹²¹Sb Mössbauer spectroscopy. The crystal structure indicated that both Sb³⁺ and Sb⁵⁺ are substituted for Sn⁴⁺ in the SnO₂ structure, Sb³⁺ being dominant for the as-prepared samples. In

annealing up to 550 °C, the Sb³⁺/Sb⁵⁺ content ratio decreased, indicating oxidation of Sb³⁺. It was found that the Sb³⁺/Sb⁵⁺ content ratio in ATO samples is proportional to the ratio of full-width at half-maximum (FWHM) for the diffraction lines 110 and 101 of these samples (B. Gržeta et al., In Cristalogafia. Fundamentos, Técnicas y Aplicaciones, Ed. L. Bucio, Sociedad Mexicana de Cristalografía A. C., México D. F. 2005: 69).

Forming of the Centre for diagnostics of Fish, Shellfish and Crustaceans Diseases

Research carried out in 2005 revealed standard values of haematological and biochemical parameters for several fish species (Oncorhynchus kisutch, Dicentrarchus labrax, Mugill spp., Thunnus thynnus). The alterations of these factors in response to some abiotic factors have been established. Comparison of the farmed and wild sea bream populations in the Adriatic Sea proved that the farming environment impacts the modification of biochemical blood parameters, decreasing the resistance of the organisms and increasing their susceptibility to bacterial, viral and parasitic diseases. The results demonstrated significant differences in biochemical and histological profiles of the free-living and farmed sea bass (R. Čož-Rakovac et al., Veterinary Research Communications 2005: 29-8: 677).

PROJECTS

Projects supported by the Ministry of Science, Education and Sport (MZOŠ)

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

INVITED LECTURES

1. Maria Ranogajec-Komor: Status and Perspectives of Dosimetry in Europe. Chiyoda Technol Corporation, Tokyo, Japan, 7.2.2005.
2. Branko Vekić: Calibration Standards for Radiation in Croatia. Chiyoda Users' Conference, Mito, Japan, 8.2.2005.
3. Maria Ranogajec-Komor: Thermoluminescence Dosimetry. Kyoto University, Kyoto, Japan, 10.2.2005.
4. Saveta Miljanić: Research and Development of Dosimetry at the Ruđer Bošković Institute. Kyoto University, Kyoto, Japan, 10.2.2005.
5. Dušan Ražem: Radiation Sterilization of Pharmaceuticals. International Atomic Energy Agency Consultants Meeting on Trends in Radiation Sterilization and Decontamination of Pharmaceuticals, Cairo, Egypt, 15. – 18. 5. 2005.
6. Dušan Ražem: Radiation Sterilization of Cosmetics. International Atomic Energy Agency Consultants Meeting on Trends in Radiation Sterilization and Decontamination of Pharmaceuticals, Cairo, Egypt, 15. – 18. 5. 2005.
7. Biserka Gržeta, Structural Studies of Nanocrystalline Sb-Doped SnO₂, plenary lecture at Quinto Congreso Nacional de Cristalografía, Guanajuato, Mexico, November 13-18, 2005.
8. Biserka Gržeta, Structural Studies of Nanocrystalline Antimony-Doped Tin Oxide (ATO) from RT to 550 °C, Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional, Mexico D. F., Mexico, 11 November 2005.

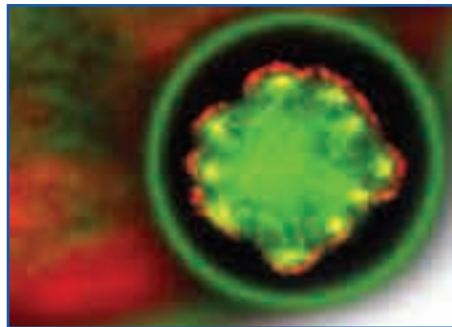
AWARDS

Damir Kralj, Marko Ukrainczyk, Jasminka Kontrec, Vesna Babić-Ivančić and Ljerka Brečević were awarded the Golden Arca (Zlatna Arca) and the Genius Cup (The Association of Hungarian Inventors) at the 3rd ARCA - International Exhibition of Innovations, Zagreb, 2005 - for the invention of VIKER.

SELECTED PUBLICATIONS

1. Bosnar S, Bronić J, Krznarić I, Subotić B. Influence of concentrations of aluminium and silicon in the liquid phase on the growth kinetics of zeolite A and X microcrystals. *Croat Chem Acta* 2005: 78: 1.
2. Štefanić G, Musić S, Trojko R. The influence of thermal treatment on the phase development in $\text{HfO}_2\text{-Al}_2\text{O}_3$ and $\text{ZrO}_2\text{-Al}_2\text{O}_3$ systems. *J Alloys Comp* 2005: 388: 126.
3. Kontrec J, Babić-Ivančić V, Brečević Lj. Formation and morphology of struvite and newberyite in aqueous solutions at 25 and 37 °C. *Coll Antropol* 2005: 29: 289.
4. Denac M, Šmit I, Musil V. Polypropylene/talc/SEBS (SEBS-g-MA) composites. Part 1: Structure. *Composites A* 2005: 36: 1094; and .Denac M, Musil V, Smit I. Polypropylene/talc/SEBS (SEBS-g-MA) composites. Part 2: Mechanical properties. *Composites A*, 2005: 36: 1282.
5. Bououdina M, Šorgić B, Ouladdiaf B, Skryabina N, Fruchart B. Neutron diffraction investigations and magnetic properties of $\text{RENi}_3.5\text{Al}_{1.5}$ Compounds and their Hydrides. *J Alloys Compd* 2005: 404-406: 64.
6. Planinić P, Rastija V, Perić B, Giester G, Brničević N. Synthesis and crystal structure of $2[(\text{Ta}_6\text{Cl}_{12})\text{Cl}_3(\text{n-BuCN})_3] \cdot [(\text{Ta}_6\text{Cl}_{12})\text{Cl}_4(\text{n-BuCN})_2] \cdot \text{n-BuCN}$, the first cluster compound containing $[\text{Ta}_6\text{Cl}_{12}]^{3+}$ and $[\text{Ta}_6\text{Cl}_{12}]^{4+}$ cores. *Comptes Rendus Chimie* 2005: 8: 1766.
7. Čož-Rakovac R, Strunjak-Perović I, Hacmanjek M, Topić Popović N, Lipej Z, Šošarić B. Blood chemistry and histological properties of wild and cultured sea bass (*Dicentrarchus labrax*) in the North Adriatic Sea. *Veterinary Research Communications*, 2005: 29: 677.

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

OVERVIEW OF THE DIVISION

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

In 2005, members of the Division of Molecular Biology participated in teaching more than 30 subjects at Croatian universi-

ties. 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.metode.avalon.hr>).

TOP ACHEIVEMENTS

DNA repair

Just 10 copies of RecBCD enzyme present in *Escherichia coli* initiate a vast majority of homologous recombination in that organism. We have shown that even a moderate increase in concentration of RecBCD enzyme in a cell reduces the efficiency of both DNA repair and homologous recombination. These results suggest that the efficient DNA recombination and repair requires balanced concentrations and fine regulation of recombination functions in the cell (D. Đermić et al., *Res Microbiol* 2005: 156: 304).

Recombination machinery

Recently, we have shown that elements of two independent recombination machineries in *E. coli* (RecBCD and RecF) can interact and together produce recombinogenic filament. We now present the genetic

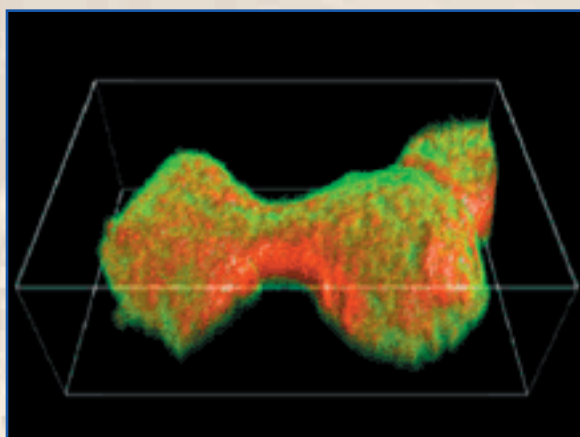


Figure 1: Three-dimensional reconstruction of a dividing cell.



Figure 2: Confocal microscope at the Division of Molecular Biology

analysis of another hybrid recombination pathway which operates in the *recB1080 recD* double mutant (I. Ivančić-Baće et al., *J Bacteriol* 2005: 187: 1350).

RNA-mediated gene regulation

Molecular biologists have been amazed in recent years by the discovery of RNA-mediated mechanisms of gene regulation. Non-coding RNAs deriving from satellite DNAs have been suggested to play a fundamental role in gene regulation being involved in epigenetic chromatin modulation, transcription, RNA maturation and translation. A review article addressing this new and exciting field of research was published in 2005 (Đ. Ugarković *EMBO Rep* 2005: 6: 1035).

Telomere shortening in senescent cells

It has been suggested that senescence is regulated by telomere shortening in human cells. We demonstrate that telomeres of early-senescent cells are the same length, and must shorten at the same rate, as cycling sister cells in the culture. These results support model of abrupt telomere shortening as a cause of sudden and stochastic nature of

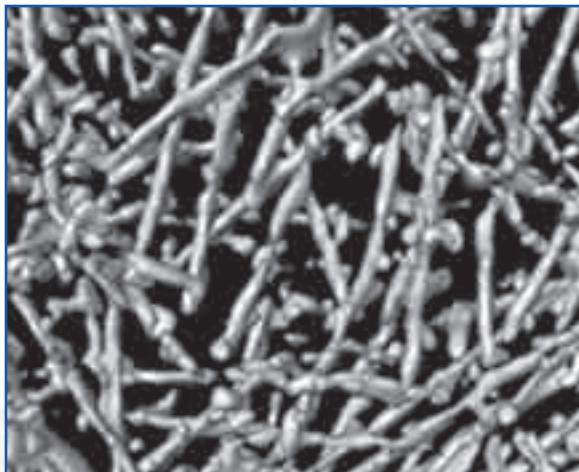


Figure 3: Electron microtomography of the actin cytoskeleton

cellular aging (M. Ferenac et al. J Gerontol Biol Sci 2005: 60A: 820).

Evolutionary population genetics

A novel concept for the origin and maintenance of adaptive genetic variation is introduced in this theoretical paper. It is based on neutral polymorphism on quantitative trait loci and on the both adaptive and neutral gene substitutions. This model can explain the fast evolution of non-essential genes and the appearance of evolutionary innovation (K. Brčić-Kostić, Genet Res 2005: 86: 53).

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

1. The role of recombination in DNA repair and genome stability, Salaj-Šmic E
2. Regulation of recombination and recombinational repair, Petranović M
3. Genes and genomes of evolutionary conserved and economically important species, Gamulin V
4. Evolutionary dynamics of satellite DNAs, Ugarković Đ

5. Organization of heterochromatic DNA sequences in invertebrates, Plohl M
6. Transcriptional regulation in eukaryotes, Sopta M
7. Molecular mechanisms of immortalization and cellular aging, Rubelj I
8. Structure, function and regulation of plasminogen serine proteases, Brdar B
9. Cell response to physical, chemical and biological noxa, Osmak M
10. Molecular pathophysiology of serotonergic transmission, Jernej B
11. Hydrodynamics of the cerebrospinal fluid, Orešković D
12. Structure and function of plastids and cytoskeleton, Ljubešić N
13. Dynamics and genetics of bioactive molecules, Magnus V
14. Endemic and relict phytocenoses of Croatia and their mycoflora, Lovrić AŽ

Other projects

1. Biodiversity in Croatia: genetic characterization of autochthonous flora and fauna and economically important species and breeds. Gamulin V, collaborative project (2003-).
2. Biological response to damage. Osmak M, collaborative project MESS (2003-).
3. Usage of telomerase in revitalization of cells and tissues in vitro and in vivo. Rubelj I, collaborative project (2003-).
4. Plant hormones – Physiology, Biochemistry and application. Magnus V, collaborative project (2003-).
5. New potential anti-cancer drugs: diazenes and triazenes. Osmak M, Polanc S (Faculty for Chemistry and Chemical Technology, University of Ljubljana), bilateral collaboration.
6. Molecular enzymology and enzyme engineering of hydrolases. Vujaklija

- D, Schwab H (Graz University of Technology), bilateral project.
7. Comparative study of distribution, structure and evolution of satellite DNA sequences in the genome of root-knot nematodes in relation with their mode of reproduction. Plohl M, Castagnone-Sereno P, Cogito bilateral project.
 8. Genetic diversity and evolutionary processes of irises along the Dinaric Alps. Fulgosi H, Till-Bottraud I (UJF Grenoble, France), Cogito bilateral project.
 9. Serotonin and impulsive behavior. Jernej B, Laviola G (Institute of Health, Roma, Italy), bilateral project.
 10. Pathophysiology of synaptic transmission: studies on an original animal model. Jernej B, Živin M (University of Ljubljana, Slovenia), bilateral project.

INVITED LECTURES

1. Weber I. Cryoelectron tomography: zooming into intact cells. Regional Biophysics Meeting, Zreče, Slovenia.
2. Weber I. Premature exocytosis in Dictyostelium discoideum cells that lack myosin II. 7th Multinational Congress on Microscopy, Portorož, Slovenia.
3. Zahradka K. Deinococcus radiodurans: the most efficient DNA repair involves coupled replication and recombination processes. 1st Central European Forum for Microbiology (CEFOM), Keszthely, Hungary.

SELECTED PUBLICATIONS

1. Brčić-Kostić K. Neutral mutation as the source of genetic variation in life history traits. Genet Res 2005: 86: 53.
2. Đermić D, Halupecki E, Zahradka

- D, Petranović M. RecBCD enzyme overproduction impairs DNA repair and homologous recombination in *Escherichia coli*. Res Microbiol 2005: 156: 304
3. Ferenac M, Polančec D, Huzak M, Pereira-Smith OM, Rubelj I. Early-senescing human skin fibroblasts do not demonstrate accelerated telomere shortening. J Gerontol Biol Sci 2005: 60A: 820.
4. Fulgosi H, Lepeduš H, Cesar V, Ljubešić N. Differential accumulation of plastid preprotein translocon components during spruce (*Picea abies* L. Karst.) needle development. Biol Chem 2005: 386: 777.
5. Hranilović D, Čičin-Šain L, Bordukalo-Nikšić T, Jernej B. Rats with constitutionally upregulated/downregulated platelet 5HT transporter: Differences in anxiety-related behavior. Behav Brain Res 2005: 165: 271.
6. Ivančić-Baće I, Salaj-Šmic E, Brčić-Kostić K. Effects of recJ, recQ and recFOR mutations on recombination in nuclease-deficient recB recD double mutants of *Escherichia coli*. J Bacteriol 2005: 187: 1350.
7. Mravinac B, Plohl M, Ugarković Đ. Preservation and high sequence conservation of satellite DNAs suggest functional constraints. J Mol Evol 2005: 61: 542.
8. Petrović V, Plohl M. Sequence divergence and conservation in organizationally distinct subfamilies of *Donax trunculus* satellite DNA. Gene 2005: 362: 37.
9. Ugarković Đ. Functional elements residing within satellite DNAs. EMBO Rep 2005: 6: 1035.

Division of Molecular Medicine



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

DIVISIONAL ORGANISATION

Head: Krešimir Pavelić

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

- ⇒ Laboratory of cellular and molecular immunology, Mariastefania Antica
- ⇒ Laboratory of molecular oncology, Jasminka Pavelić
- ⇒ Laboratory of molecular pathology, Koraljka Gall-Trošelj
- ⇒ Laboratory of experimental hematology, immunology and oncology, Jelka Gabrilovac
- ⇒ Laboratory of biological response modifiers, Tatjana Marotti
- ⇒ Laboratory of immunochemistry, Biserka Pokrić
- ⇒ Laboratory of molecular endocrinology and transplantation, Mirko Hadžija
- ⇒ Laboratory for oxidative stress, Neven Žarković
- ⇒ Laboratory of molecular neuropharmacology, Danka Peričić
- ⇒ Laboratory of functional genomics, Marijeta Kralj
- ⇒ Laboratory of molecular virology and bacteriology, Magdalena Grce
- ⇒ 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 disease and to develop and improve new strategies for the diagnosis, treatment and prevention of disease. These goals are realized through the evaluation of the impact of genetic factors in disease prevention, the reduction of risk factors, the development and evaluation of new drugs, the exploration of the biochemical and cellular effects of drugs on cells and living organisms, the improvement of scientific methodology, and the education of scientists and students.

The Division is currently developing several strategic projects. These include the development of molecular targeted therapy for use against cancer and viral diseases, new diagnostic tools and research aimed at deciphering the molecular basis of disease, tools based on transcriptomic and proteomic approaches, as well as tissue engineering for the purpose of therapeutic cloning. As such, the Division is emerging as a pre-eminent centre (centre of excellence), for research in molecular approaches to the study of disease.

TOP ACHIEVEMENTS IN BASIC RESEARCH

S-Adenosylhomocysteine hydrolase (SAHH) deficiency in human

DNA analysis of patients showed a total of 5 different as yet uncharacterized point mutations in the SAHH gene. The severity of the disease is variable and causes serious health problems with a possible lethal outcome if some of the point mutations occur in combination. So far we have characterized one missense mutation in detail, which represents a temperature sensitive mutation as confirmed by circular dichroism analysis. The catalytic rates of mutant protein are decreased to approximately 30% of normal. The reason for reduced enzyme activity is linked to the oxidation states of bound co-factor NAD. Thus, mutant protein contains mainly NADH, which means that protons usually bound by NAD^+ and obligatory for substrate oxidation are not retained in the active site, i.e. causing reduced enzyme activity and therefore SAHH deficiency in human (I. Barić et al., J Inher Metab Dis 2005: 28:885).

Optimization procedure for the best selection of ligand-receptor

An optimization procedure for the best selection of ligand-receptor pairs is derived from the Molecular Recognition Theory (MRT). The MRT is based on the finding that peptides specified by the complementary RNAs bind to each other with higher specificity and efficacy. The theory was investigated considering the interaction of the sense peptides coded by means of messenger RNA (read in 5' -3' direction) and

antisense peptides coded in 3' -5' direction. The hydrophathy of the complementary amino acid pairs and their frequencies in 10 peptide-receptor systems with verified ligand-receptor interaction was analysed. The MRT was validated by "in vivo" experiment as an useful method to simplify experimental procedures, reduce the costs of the peptide synthesis, and improve peptide structure modelling (N. Štambuk et al., Theor Biosci 2005: 123: 265).

The role of NF1 gene in the development and progression of colon cancer

Real-time RT-PCR was used to determine NF1 mRNA expression in tumours and corresponding normal mucous tissue. The relative ratio of NF1 mRNA type I and II isoforms expression was examined as well. NF1 gene expression was significantly increased in tumour tissue compared to corresponding normal tissue. There was a statistically significant increase of NF1 mRNA type I isoform expression in tumour tissue when compared to corresponding normal colon tissue. NF1 might play a role in the development and progression of colon cancer and this gene could be a potential target for therapy (an extensive comment of these results was published in Nature Clinical Practice 2005: 2:542).

Molecular mechanisms of immunosuppression

The down regulation in interferon alpha and gamma transcription following exposure to a very virulent strain of Marek's disease virus as opposed to a vaccinal strain has been observed in B(13)/B(13) chickens. This result has implications to the disease's

role in immunosuppression and the virus's oncogenicity (P. Quere et al., Arch Virol 2005: 150:507). The enhanced flow through kynurenine pathway of tryptophan degradation has been proven to up regulate transcription of inducible nitric oxide synthase in chicken macrophages.

TOP ACHIEVEMENTS IN APPLIED RESEARCH

A novel therapeutic indication

A new pharmacotherapeutic strategy for combat exposed war veterans with psychotic PTSD, refractory to prior antidepressant treatment, was confirmed by N. Pivac and her colleagues. Atypical antipsychotic drug risperidone significantly reduced psychotic and PTSD symptoms in psychotic PTSD patients, corroborating the hypothesis that atypical antipsychotics might be the drugs of choice in treatment-resistant patients with psychotic combat related PTSD (D. Kozarić-Kovačić et al., J Clin Psychiatry 2005: 66: 922). The significance of the article was shown in its brief description in Psychiatry source, Psychiatry Matters and in Doctor's guide.

Biological markers

The hypothesis that platelet monoamine oxidase (MAO) is a biological marker for alcoholism was questioned by N. Pivac et al. (Psychopharmacology 2005: 182: 194). They found that platelet MAO activity was not reduced in an ethnically homogenous group of drug-free alcoholic subjects when compared to healthy controls, and that the differences in platelet MAO activity were related to sex and smoking status of subjects.

Antiviral effect of clinoptilolite

A New approach for antiviral drug testing has been proposed based on the in vitro model with human adenovirus type 5, herpesvirus type 1, coxsackie virus Cocksackievirus B5 and echovirus 7. Our results indicate a possibility of therapeutical application of clinoptilolite either locally (skin) against herpes virus infections, or orally in cases of adenovirus or enterovirus infections (M. Grce and K. Pavelić, Micropor Mesopor Mater 2005: 79:165).

New analytical method

In 2005 the Laboratory for Oxidative Stress published a genuine method for the immuno-electronmicroscopy (immunogold) of 4-hydroxynonenal-histidine conjugates,

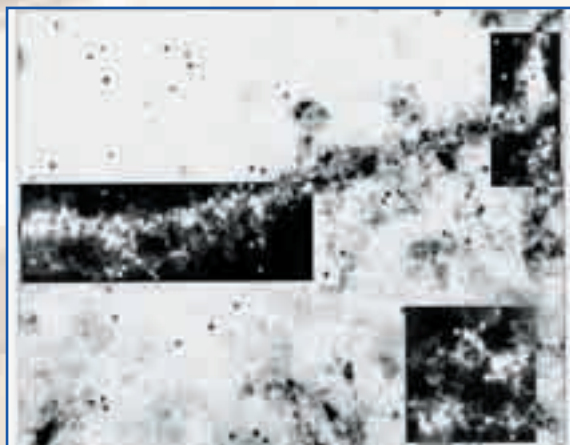


Figure 1: Electron microscopic analysis of 4-hydroxynonenal (HNE)-treated peripheral blood leukocytes of Wistar rat (marked by 10-nm colloidal gold particles). Genuine monoclonal antibodies against HNE-histidine show remarkable immunopositivity mostly in damaged membrane structures and in the vicinity of cellular membranes in the cytoplasm (magnification 71 000). This proves that not only is endogenous HNE generated during lipid peroxidation but also that exogenously added aldehyde is mostly bound to the membranous structures acting as a "second messenger of free radicals" and a mediator of lipid peroxidation (M. Živković et al., Croat Chem Acta, 2005: 78: 91).

which may be used as an analytical immunochemical method to study lipid peroxidation in pathological and physiological processes and for pathomorphological diagnostic procedures. We published four invited articles in the journal *Biofactors*, describing genuine findings on cellular and molecular aspects of lipid peroxidation, such as the relationship between 4-hydroxynonenal and the level of differentiation (malignancy) of malignant cells as well as effects of inflammatory cells on the growth of normal and malignant cells.

Therapeutical cloning

Experiments toward therapeutic cloning of pancreatic Langerhans islets have also been successfully conducted in 2005. Figure 3 shows five-stage procedure of the embryoid bodies development for the cell therapy of diabetic recipients.



Figure 2: Mouse oocyte fertilization in vitro

New clinical studies

Three clinical studies in the field of digestive disorders were published that described: 1) the relationship between the expression of TfR1 or ferritin and the grade of colorectal carcinoma, 2) the differential pattern of oxidative stress in patients treated by open and those treated by laparoscopic surgery and 3) the effectiveness of the perioperative use of the Viscum album drug Isorel to attenuate side effects of surgery in patients with digestive carcinomas.

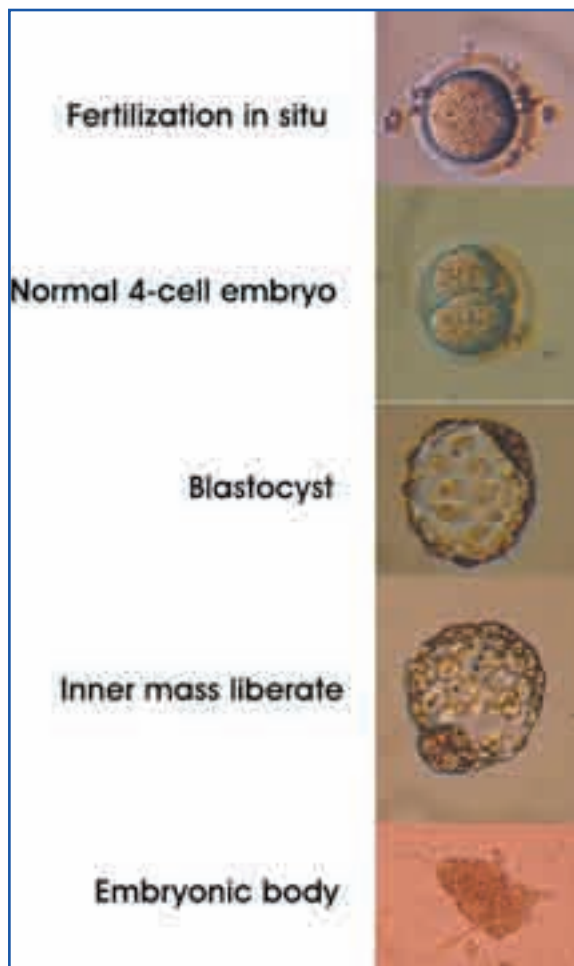


Figure 3: Therapeutical cloning of pancreatic Langerhans islets

Screening of newly synthesized anticancer compounds

Over 200 newly synthesized compounds were screened in vitro for potential anti-tumor activity, such as cyano- and isopropylamidino-substituted derivatives of benzo-carboxanilides and benzo-quinolones, derivatives of hydroxyurea and hydantoins, as well as a novel amidino-substituted naphthofuran-methyl-carboxylate. The possible mechanisms of action were ascertained for the most effective ones.

MODERN FACILITIES, METHODS AND EQUIPMENT

Proteomic unit

The Proteomics Unit has recently been additionally equipped with an imaging system – VersaDoc 4000 (BIO-RAD). VersaDoc is a quantitative imaging system capable of capturing high resolution digital images from single and multi-colour fluorescence, chemiluminescence, chemifluorescence, white light and colorimetric samples. Its current application encompasses chemiluminescent western blots and cDNA array imaging as well as imaging of Coomassie Blue-stained or silver-stained 2-DE gels. VersaDoc is directly connected with a Personal Computer with two specialized software packages for protein analyses, namely Quantity One 1-DE analysis software and PDQuest 2-DE analysis software. Quantity one is mainly being used for molecular weight determination and quantitation of protein samples while PDQuest proved successful in identification of differences in protein expression.



Figure 4a: VersaDoc imaging system

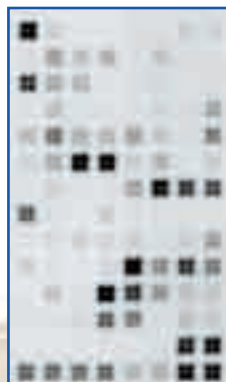


Figure 4B

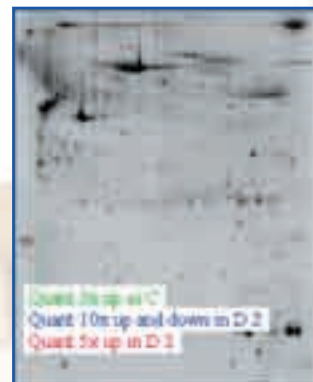


Figure 4C

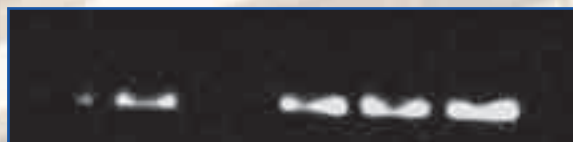


Figure 4D

DNA-chip, 2-DE gel and nitrocellulose membrane from Western blot analysis scanned by the VersaDoc imaging system (BIO-RAD, USA)

Test for hereditary breast cancer

The high resolution melting approach for rapid mutation (or polymorphic) screening and detection was introduced recently. Conventional mutation scanning methods require a separation step and include single strand conformational polymorphism (SSCP) analysis, heteroduplex analysis, denaturing gradient gel electrophoresis or denaturing HPLC. Subsequently, these methods require separation of PCR products on a gel or other matrix, often taking more time to perform. Taking advantage of the high resolution melting approach, the HR-1 High resolution melter apparatus from Idaho Technology was used. The HR-1 works in combination with adapted Rapid Cycler (Thermocycler) and fluorescent dye LC Green Plus. LC Green Plus during PCR reaction incorporates into ds DNA, showing different melting profile and fluorescence (450 nm excitation/470 nm emission), during heating from, i.e. 60⁰ to 95⁰ C reflecting polymorphic or mutational variability.

High-resolution melting analyses data for polymorphisms of BRCA1 gene involved in hereditary breast cancer.

Results are expressed as a melting curve (fluorescence vs temperature) or it's derivative plot ($-dF/dT$ vs. temperature) or a difference plot (fluorescence vs. temperature).

Every coloured curve represents an individual unique variant sample. Those samples appearing in clusters need to be confirmed by sequencing.

The model of molecular diagnostic of nonsyndromic hearing loss was established.

Figure 5: BRCA 1 exon 17 – four samples showing two patterns.

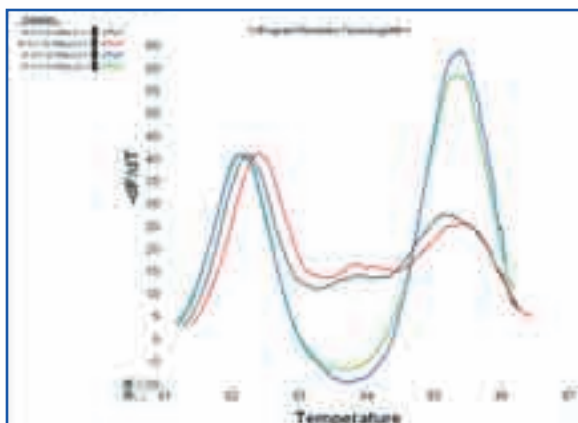


Figure 5a: BRCA 1 exon 17 – melting curve

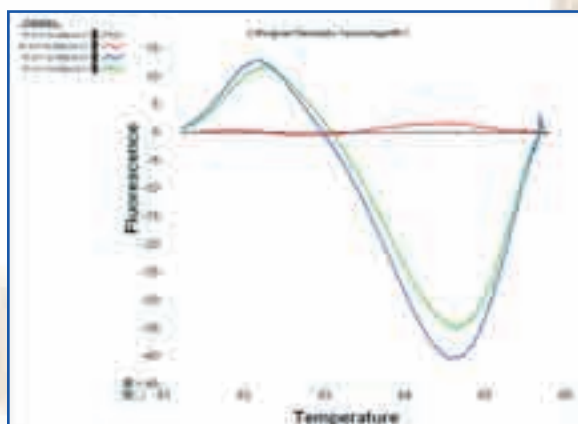


Figure 5b: BRCA 1 exon 17 – derivative plot

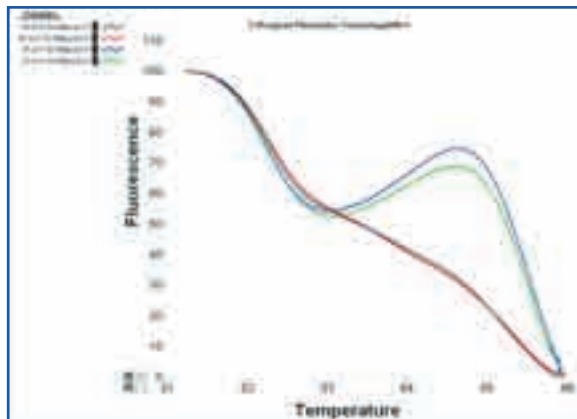


Figure 5c: BRCA 1 exon 17 – difference plot

New equipment

- BioRobot EZ1 Workstation for low-throughput nucleic acid purification from a wide range of biologically relevant samples
- Low pressure liquid chromatography system
- VersaDoc imaging system
- High resolution melter apparatus. The HR-1 works in combination with adapted Rapid Cycler (Thermocycler) and fluorescent dye LC Green Plus.

Education

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

AWARDS

1. Award to Dorotea Muck-Šeler: The Croatian State Reward, the most prestigious scientific recognition available in Croatia, was given to Dorotea Muck-

Šeler, senior research scientist at the Division of Molecular Medicine. Dorotea Muck-Šeler was awarded for the research in biological psychiatry, on the peripheral serotonergic markers of psychiatric disorders, and the role of serotonin in the ethiopathogenesis of psychiatric disorders.

2. Award to Milivoj Boranić: The Croatian State Reward for life achievement in biomedicine. Professor Milivoj Boranić was awarded for his contribution in bone marrow transplantation and leukaemia research.

PROJECTS

Projects supported by the Ministry of Science and Technology (MZT)

1. Molecular mechanisms in the pathogenesis of neuroendocrine tumours, Koraljka Gall-Trošelj
2. Molecular genetics of gastrointestinal tumours, Sanja Kapitanović
3. The SHH/PTCH/SMO signalling pathway in cancer and development, Sonja Levanat
4. Role of FHIT in neuroendocrine tumours, Šime Križanac
5. Insulin-like growth factor family of genes in lung cancer, Ljubomir Pavelić
6. New therapeutic possibilities in breast cancer, Josip Unušić
7. Genetic and molecular prognostic factors of cervical cancerogenesis, Magdalena Grce
8. Oxidative stress and malignant diseases, Neven Žarković
9. Gene or protein transduction and signalling pathways in transformed cells, Krešimir Pavelić
10. Cyclooxygenase-2: new target for

chemoprevention and treatment of colon tumours, Radan Spaventi

11. Molecular mechanisms of immuno-suppression, Renata Novak
12. Modulation of immunological response by bioactive peptides, Biserka Pokrić
13. Transcriptional control of lymphocyte development – its role in leukemogenesis, Mariastefania Antica
14. Tumour gene therapy – correction of oncosuppressor genes, Jasminka Pavelić
15. Virus antitumorous action and oncolytic virus vaccine, Mislav Jurin
16. Embryonic cell production of pancreatic-like islets, Mirko Hadžija
17. DNA chip technology in global profiling of tumours, Šime Spaventi
18. Nonlinear modulation of the chronic lymphatic leukaemia, Branko Vitale
19. Regulation of ectopeptidases and opioid receptors expression, Jelka Gabrilovac
20. Oxidative/antioxidative status after treatment with opioids/opiates, Tatjana Marotti
21. Neuropharmacology of serotonergic system, Dorotea Mueck-Šeler
22. Neurotransmitters in stress and regulation of GABA-A receptors in vitro, Danka Perićić
23. Assessing functions of the heat repeat in Huntington protein, Oliver Vugrek
24. The effects of new drugs and hyperthermia on the growth of mouse tumours and human xenografts, Marko Radačić
25. Immune interactions and immunomodulation in genital herpes infection, Zorka Mikloška

Research and development projects

1. Centre for integrative genomics, molecular diagnostics, cellular and gene therapy, Krešimir Pavelić (MZOŠ, JEZGRA, J-1-2004)
2. Development of new analgetic, antirheumatic and antioxidative substances from pine resin, Neven Žarković (MZOŠ, HITRA, TP-01/0098-28)
3. Development of a new and improved vaccine against genital herpes, Zorka Mikloška (MZOŠ, HITRA, TP-03/0098-39)
4. Molecular genetic background of Gorlin syndrome, Sonja Levanat (Bilateral Cooperation "Cogito", Bordeaux, France)
5. Developing method for detection of inherited predisposition to breast cancer in Croatia, Sonja Levanat (MZOŠ, HITRA, TP-07/009840)
6. Application of macromolecular derivative (G-90) from *Eisenia foetida* in biomedicine, Mira Grdiša (MZOŠ, HITRA, TP-03/009841)
7. Involvement of the ESCRT machinery in TfR sorting towards HD3 exosomes. Mira Grdiša (Cogito)
8. Bioactive properties of domestic pollen from *Salix alba* and *Cistus* sp. Tanja Marotti (HITRA, TP-05/0098-49).
9. The role of cholesterol in Alzheimer's disease, Silva Hećimović (Fogarty International Research Collaboration Award- NIH, USA, 1R03TW007335-01)

In 2005 our proposal for the new COST (European Cooperation in the field of Scientific and Technical Research) Action B35 "Lipid Peroxidation Associated Disorders" was accepted as the only new priority in the field of Medicine and Health. The B35 Action is scheduled to become operative in 2006 and

will be the only COST Action coordinated by Croatia in all COST domains.

Other projects

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

SELECTED LECTURES

1. Pivac N, Kozarić-Kovačić D, Mück-Šeler D: Biological markers in Croatian war veterans with combat related posttraumatic stress disorder, in NATO programme security through science advanced research workshop: Novel Approaches to the Diagnosis and Treatment of Posttraumatic Stress Disorder, Cavtat, Croatia, June 13-16, 2005.
2. Pavelić K: Nanomedicine - Medicine on a small scale. Plenary lecture. Nanotechnology, Drug Delivery System. Chiang Mai, Thailand, February 21-22, 2005.
3. Pavelić K: Accelerating drug discovery: The role of omics technology. Plenary lecture. Free Radical School. Chiang Mai, Thailand, February 21-22, 2005.
4. Pavelić K: Aggressive and criminal behaviour, molecular medicine and new judicial system. "Medicine and Law". Maribor, Slovenia, March 18-19, 2005.
5. Pavelić K: Strategies for supporting life sciences research in scientifically developing countries in Europe. EMBC/EMBO Workshop on Advancing life sciences research in Europe. Berlin, Germany, April 18, 2005.
6. Pavelić K: Omics revolution in medicine: The second generation will benefit from

- breakthrough in science. 13th Congress of European Union for School and University Health and Medicine Dubrovnik, Croatia, October 12-15, 2005.
7. Pavelić K: Cancer Research meets functional genomics – what has been accomplished so far? Molecular Diagnostic in Medicine. Ljubljana, Slovenia, November 30 - December 2, 2005.
 8. Grce M: Genital HPV infection: Health implication and diagnosis. 1st Central European Forum for Microbiology, Keszthely, Lake Balaton, Hungary, October 26-28, 2005
 9. Pavelić J: Tools for molecular diagnostics. 5. Bednjaničev simpozij: Nalezljive bolezni v otroški dobi., Maribor, Slovenija, May 27-28, 2005.
 10. Lavanat S: Hedgehog-Patched alterations in different tumors and malformations, Inaugural meeting: Hedgehog – Gli signalling in Development and Disease European Network, Sponsored by Louis-Jeantet Foundation and the NCCR-Frontiers in Genetics, Geneva, July 7, 2005.
 11. Lavanat S: Role of the Hedgehog/Patched signalling pathway in oncogenesis. Alterations of PTCH are attributed to the pathway activation in ovarian fibromas and dermoids, 10th World Congress on Advances in Oncology and 8th International Symposium on Molecular Medicine. Creta, October 13-15, 2005.
 2. Kraljević S, Pavelić K: Navigare necesse est. EMBO Rep 2005; 6 : 695.
 3. Pavelić K, Etra A, Gall-Trošelj K: Insights from the front lines of nutraceutical research: The Third International Conference on Mechanisms of Action of Nutraceuticals (ICMAN 3). J Altern Complem Med 2005; 11: 735.
 4. Grce M: Cervical cancer and human papillomavirus. BJMG 2005; 8: 19.

Additional publications

1. Kozarić-Kovačić D, Pivac N, Muck-Šeler D, Rothbaum BO: Risperidone in psychotic combat related posttraumatic stress disorder: an open trial. J Clin Psychiatry 2005; 66: 922.
2. Pivac N, Muck-Šeler D, Kozarić-Kovačić D, Mustapić M, Nenadić-Šviglin K, Deželjin M: Platelet monoamine oxidase in alcoholism. Letter to the Editors. Psychopharmacology 2005; 182: 194.
3. Jarak I, Kralj M, Šuman L, Pavlović G, Dogan J, Pavelić K, Karminski-Zamola G: 2-carboxanilides and benzo(b) thieno(2,3-c)quinolones: synthesis, photochemical synthesis, crystal structure determination and antitumor evaluation. Part 2. J Med Chem 2005; 48: 2346.
4. Opačić N, Barbarić M, Zorc B, Cetina M, Nagl A, Frković D, Kralj M, Pavelić K, Balzarini J, Andrei G, Snoeck R, De Clercq E, Raić-Malić S, Mintas M: The novel L- and D-amino acid derivatives of hydroxyurea and hydantoins: synthesis, X-ray crystal structure study, cytostatic and antiviral evaluations. J Med Chem 2005; 48: 475.
5. Pavelić J, Križanac Š, Kapitanović S, Pavelić LJ, Samaržija M, Pavičić F, Spaventi Š, Jakopović M, Herceg-Ivanović Z, Pavelić K: The consequences of insulin-like growth factors/receptors dysfunction.

SELECTED PUBLICATIONS

Review articles

1. Kralj M, Kraljević S, Sedić M, Kurjak A., Pavelić K: Global approach to perinatal medicine: functional genomics and proteomics. J Perin Med 2005; 33 : 5.

- tion in lung cancer. *Am J Respir Cell Mol Biol* 2005; 32: 65.
6. Barbarić M, Uršić S, Pilepić V, Zorc B, Hergold-Brundić A, Nagl A., Grdiša M, Pavelić K, Snoeck R, Andrei G, Balzarini J, DeClercq E, Mintas M: Synthesis, X-ray cristal structure study, cytostatic and antiviral evaluation of the novel cycloalkyl-N-aryl-hydroxamic acids. *J Med Chem* 2005; 48:884.
 7. Čačev T, Radošević S, Spaventi R, Pavelić K, Kapitanović S: NF1 gene loss of heterozygosity and expression analysis in sporadic colon cancer. *Gut*, 2005; 54:1129.
 8. Čupić B, Breljak D, Gabrilovac J: Receptor-mediated down-regulation of neutral endopeptidase (NEP; EC 3.4.24.11, CD10) on immature B lymphocytes by dexamethasone. *Int J Mol Med* 2005; 15: 1023.
 9. Prutki M, Poljak-Blazi M, Jakopovic M, Tomas D, Stipancic I, Zarkovic N: Altered iron metabolism, transferrin receptor 1 and ferritin in patients with colon cancer. *Cancer Letters* 2005 Aug 16; [Epub ahead of print]
- NY : Nova Science Publishers, Inc., 2005. pp. 29-53.
 2. Moll UM, Slade N: The role of p53 and p73 genes in tumor formation. In: *Handbook of Immunohistochemistry and in situ hibridization of human carcinomas*. Vol 3: Molecular Genetics: Liver Carcinoma and Pancreatic Carcinoma. Ed. Hayat M.A., SAD : Academic Press, 2005. pp 103-117.
 3. Gabrilovac J, Čupić B, Breljak D, Kraus O, Jakić-Razumović J: Expression of membrane peptidases on cultured human keratinocytes. In: *Progress in Immunology Research*. Ed: Veskler B.A.. New York : Nova Science Publishers, 2005, pp.83-105.
 4. Žarković N.: Mechanismen der Tumorentstehung. In: *Oxidativer Stress und Pharmaka* Eds: Werner S, Krämer K, Grune Tilman. Govi-Verlag, Eschborn, 2005, pp 145-158
 5. Žarković N.: Antioxidation in der Prävention und Chemotherapie von Tumoren. In: *Oxidativer Stress und Pharmaka*. Eds: Siems Werner, Krämer K, Grune Tilman, Govi-Verlag, Eschborn, 2005, pp 159-174

Chapters in books

1. Muck Šeler D, Pivac N, Šagud M, Mustapić M, Jakovljević M: The effects of serotonin uptake inhibitors on platelet serotonin: From basic to clinical research. *Trends in Serotonin uptake inhibitor research*. Chapter 2, Ed: Shirley A.C. Hauppauge,

Division of Marine and Environmental Research



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

DIVISIONAL ORGANISATION

Head: Tarzan Legović

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

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

OVERVIEW OF THE DIVISION

During 2005, scientists of the division worked on over 50 research projects contracted by the Ministry of Science, Education and Sport and by outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from interplanetary ecology and satellite oceanography, on the large scale, down to nanotechnology. Each project contributed to the overall mission of the division, which is to strive for excellence in fundamental and applied research of environmental systems, their processes, states and control. The research is directed toward an increase in the knowledge base needed for the optimum management of environment and hence the benefit of our country and, indeed, the whole world.

In 2005 scientists from our Division, in collaboration with the Institute for Oceanography and Fisheries, the Hydrographic Institute and the Fritjof Nansen Institute completed a proposal to the International Maritime Organization for declaring the Adriatic Sea as a Particularly Sensitive Sea Area. The proposal is based on the uniqueness, biodiversity and fragility of the ecosystem, human dependency, existing social, cultural, archaeological and economic values that need to be preserved. The proclamation will

constitute a legal basis for the adoption of a number of associated measures designed to decrease the likelihood of accidents, as well as to regulate and monitor ship traffic.

The research results were published in 39 scientific papers in journals indexed in Current Contents. In addition to the 15 invited lectures held in 2005, 8 conferences were organized under the auspices of the Division. Also in 2005, 3 post-graduate programs were coordinated and 13 undergraduate and 40 post-graduate courses were given at universities in Croatia and abroad.

TOP ACHIEVEMENTS

AFM imaging of the giant gel formation in the Northern Adriatic

In the field of marine biophysics, we started studying the aggregation of organic matter on the nanoscale using Atomic Force Microscopy. We systematically followed the sol-gel phase transition using field samples from the Northern Adriatic. Three principal stages in the sol to giant gel transformation were recognized (Figure 1). The results of studying marine gels on the nanoscale and the biophysical mechanism of its formation represent ground-breaking insights into the nanoscale processes and how they influence large-scale processes in the ocean (V. Svetličić et al., Ann. NY Acad. Sci. 2005: 1048: 524).

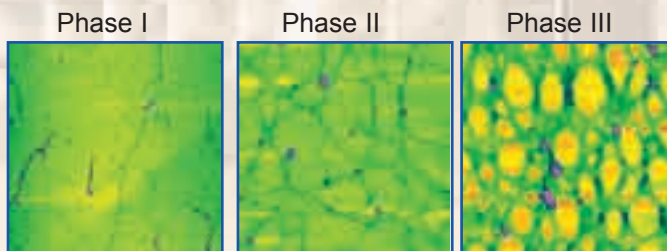


Figure 1: The first marine process studied at nanoscale: Giant gel formation in the Northern Adriatic aquatorium observed using recently installed AFM.

An improved model for prediction of the Adriatic tidal response

A very high resolution finite element model of the Adriatic Sea was implemented with a view to improve the predictions of the Adriatic tidal response. A form of variational data assimilation was employed to blend the data-derived harmonic constants and the model dynamics. A mesh of 23055 nodes and 37200 elements enabled the resolution of 77 major islands, offering better recognition of basin bathymetry, lateral geometry, improved sea-level and tidal current response (I. Janeković and M. Kuzmić. Annales Geophysicae 2005: 23: 3207).

Formation of metal sulphide nanoparticles

An association of Cu with sulphide in aerobic natural waters has been attributed to the coexistence in clusters having sizes intermediate between mononuclear complexes and colloidal particles. Copper sulphide solid phases display size-related voltammetric behaviour at Hg electrodes. Titrating Cu^{2+} into organic-rich (mucilaginous) Adriatic Sea water, which contains 10^{-7} M natural thiols and sulphide, produces solid products indicating that voltammetry might be very useful for studying the formation of semiconductor sulphide nanoparticles in nature. (I Ciglencečki et al., J Marine Sys 2005: 56: 29, I Ciglencečki et al., Environment Sci Tech 2005: 39: 7492).

Organic matter characterization in north Norwegian fjords

Organic matter (OM) distribution and its reactivity in the north Norwegian fjords were studied for the first time. General

OM parameters, dissolved and particulate organic carbon and the distribution of specific compounds such as folic acid and surface active substances, were measured using electrochemical methods developed in our institution. The distinct OM distribution in the investigated fjords indicates the potential importance of the results in this study in carbon cycling of subarctic waters (B. Gašparović et al., *Estuarine Coastal and Shelf Sc* 2005: 62: 95).

Determination of xenobiotic chemicals in wastewaters and their removal by advanced wastewater treatment

Highly specific methods based on high-performance liquid chromatography (HPLC) and tandem mass spectrometry (MS/MS) were developed for the determination of several groups of environmental contaminants, including surfactants and their endocrine-disrupting degradation products and the main classes of antimicrobials. It was demonstrated that advanced wastewater treatment using membrane biological reactors in combination with nanofiltration and advanced oxidation significantly improves the elimination efficiency of surfactants and pharmaceutical chemicals from different types of wastewaters (S. Terzić et al., *Wat. Sci. Technol.* 2005: 51: 447).

Mixed bacterial culture for atrazine degradation

The growth kinetics of microbial communities and their metabolic activities in atrazine degradation was studied within the scientific research project "Microbial communities as catalysts in biotransformation processes". As a result, a conceptual model for biotechnological treatment of atra-

zine production wastewater was developed. Patent application "Mixed bacterial culture for atrazine degradation" (no. P20060076A) submitted.

A new, non-invasive method for determination of the ABC proteins transport activity in invertebrates

In accordance with growing requests for alternate bio-monitoring techniques and a more human/rational use of experimental organisms, a new method for the determination of the expression and activity of the ABC transport proteins in haemolymph of aquatic invertebrates was developed and standardized in 2005. The method is non-invasive and allows multiple uses of the same individuals.

Uranium found in Brazilian pegmatite rock

A highlight of recent research was the finding that uranium is present in the mineral meta-autunite (found in a Brazilian pegmatite rock) in the form of uranium(V). Uranium's oxidation state 5+ is regarded as metastable and this is only the second time that such an occurrence has been described in the literature. Uranium was identified in this oxidation state by a combined electrochemical and electron paramagnetic resonance (EPR) approach. This research, done in a joint effort of 3 laboratories from 3 departments of the R. Bošković Institute and 2 other institutions in Croatia, was performed within an international collaboration between Croatia and Brazil (V. Bermanec et al. *Neues Jahrbuch fuer Mineralogie – Abhandlungen* 2005: 181: 27).

Conditions for retaining dissolved iron in aquatic solution

Dissolved iron has a crucial role in primary production processes of aquatic environment. Hence, numerous complexes of ionic iron were investigated concerning their solubility and retention in solution. A new mixed-ligand complex iron(III)-glycin-NTA, stable in the solution over 24 hours at seawater pH (~8), was determined with a concentration of iron several orders of magnitude higher than in natural waters, enhancing the iron bio-availability (V. Cuculić et al. J Electroanal Chem 2005: 583: 140).

SELECTED INVITED LECTURES

- Ahel M. Surfactant-derived alkylphenolic compounds, Analytical Sciences in Environmental and Geological Research, Duebendorf, Switzerland, 20 September 2005
- Jusup M. Impact of aquacultures on the marine ecosystem: modelling benthic carbon loading over variable depth. 5th Euro. Conf. on Ecol. Model, Pushchino, Russia, 22. September 2005.
- Klanjšček J. Is anchovy (*Engraulis encrasicolus*, L.) overfished in the Adriatic Sea?
- 5th Euro. Conf. on Ecol. Model., Pushchino, Russia, 22. September 2005.
- Kniewald G., Oceanographic research in the Adriatic sea, Croatian sector. 1st Alexander von Humboldt Research Conference on the El Nino phenomenon and its global impact, Guayaquil, Ecuador, May 2005.
- Legović T. Adriatic Sea: Why exclusive economic zones must be proclaimed. University of Innsbruck, Innsbruck, 19 October, 2005.

- Raspor, B., Fifty-five years of Ruđer Bošković Institute- continuous changes, Chemical Science and Technology Laboratory, NIST, Gaithersburg, MD, USA, 5-9. December.2005.
- Smital, T. Ecotoxicological relevance of the MultiXenobiotic Resistance (MXR) inhibitors – as a new class of hazardous chemicals among pharmaceuticals, personal care products, pesticides and other conventional pollutants, *Swiss National Research Programme 50 Seminars*, University of Zürich and University of Lausanne, Switzerland, 27.-30. April 2005
- Svetličić V, Žutić V, Durand-Vidal S. Marine Ecology at Nanoscale: Supramolecular Organization of Marine Gel. Seeing at the Nanoscale III, An International Conference. Santa Barbara, California, USA. 2005.

SELECTED ORGANIZED CONFERENCES

- Biomarkers, risk and environmental assessment. Cavtat, 6-10 April 2005. (B. Raspor)
- Eutrophication in the Coastal Zone of the Eastern Adriatic Sea. Hvar, 27 April - 1 May 2005, (B. Čosović and P. Wassmann)
- 4th Scientific Meeting of Croatian Biophysicists. Zagreb, Croatia, 9 September 2005 (V. Svetličić)
- 5th European Conference on Ecological •Modelling. Pushchino, Russia, 19-23 September 2005 (T. Legović)
- 1st International Workshop on Organic Matter Modeling, Toulon, France, 16-18 November 2005.(G. Kniewald)



Figure 2: Cover page of the 3rd SARIB Meeting at R. Bošković Institute.

PROJECTS

Projects supported by the Ministry of Science, Sport and Education

1. Tidal and longer-period dynamics of the northern Adriatic, Milivoj Kuzmić
2. Analysis and biogeochemistry of organic compounds in the aquatic environment, Marijan Ahel
3. Physical chemistry and biogeochemistry of trace metals in aquatic systems, Ivanka Pižeta
4. Nature and reactivity of organic substances in seawater and environment, Božena Ćosović
5. Electroanalytical research in liquid and solid electrolytes, Milivoj Lovrić
6. Models and info. systems for environmental protection and navigation management, Ivica Ružić
7. Protection of biocenotic balance in aquaculture receiving waters, Emin Teskeredžić
8. Preparation and properties of metal surfaces in the environmental protection, Dunja Čukman
9. Interfacial processes and eutrophication, Vera Žutić
10. Radionuclides in environmental systems, Delko Barišić
11. Metals and cellular biomarkers, Biserka Raspor
12. Persistent organohalogen pollutants in some

- coastal area of Dalmatia, Mladen Picer
13. Geochemistry of recent and ancient sedimentary systems of the Adriatic platform,
14. Goran Kniewald
15. Modelling aquatic ecosystems, Tarzan Legović
16. Microbial communities as catalysts in biotransformation processes, Dubravka Hršak
17. Multixenobiotic resistance mechanism as a biomarker of environmental quality, Tvrtko Smital

Other projects

1. **Reduction of environmental risks and health risks, posed by Emerging Contaminants, through advanced treatment of municipal and industrial wastes,** Marijan Ahel (EMCO EU-FP6)
2. Mitigation of environmental consequences of the war in Croatia – risk assessment of hazardous chemical contamination, Marijan Ahel and Goran Kniewald (Norwegian-Croatian joint project, 2002-2000)
3. Developing of field method for total alpha, radon and thoron activity measurement in soil gas, Delko Barišić (Bilateral Croatian-Slovenian project)
4. Determination of ecotoxic metals in water and sediments of NP Mljet, V. Cuculić
5. Geochemistry of ecotoxic metals in NP Krka, N. Cukrov
6. Croatian national monitoring programme, B. Ćosović et., al
7. Reference laboratory. Ministry of Agriculture, Forestry and Water Management, Water
8. Management Directorate, Božena Ćosović, Zlata Kozarac, Dubravka Hršak, Biserka Raspor
9. Ecosystem dynamics, marine chemistry, aquaculture and management in the Adriatic and
- North Norwegian coastal zone, Božena Ćosović and Paul Wassmann from the University of Tromso, Norway (Cooperation programme

- with South East Europe)
10. Conceptual model for biological treatment of effluents from atrazine production, Dubravka Hršak (HITRA)
 11. Taxonomic, genetic and physiological characterization of bacteria for atrazine degradation, Coordinator Dubravka Hršak (French-Croatian bilateral COGITO project, 2005-2006)
 12. MONALISA, The role of natural organic matter in speciation of bioavailable contaminants in coastal waters, Goran. Kniewald (French-Croatian Cooperation)
 13. Mediterranean Mussel Watch Program, Goran Kniewald and Delko Barišić (CIESM, 2002 – 2006)
 14. Environmental sono-electroanalysis: manganese speciation and determination, Šebojka Komorsky-Lovrić and R. Compton, Oxford University (The Royal Society, 2003-2005)
 15. Novel physical chemical techniques to characterize the sea surface microlayer, Zlatica Kozarac with Andrew Nelson from the School of Chemistry, University of Leeds, UK (Royal Society program)
 16. Ecosystem Approach for Sustainable Aquaculture, Tarzan Legović (ECASA, EU-FP6-2003)
 17. Adriatic as a particularly sensitive sea area, Norwegian-Croatian project (Tarzan Legović)
 18. Monitoring of Dunav water quality, S. Lulić (Croatian Water Management, 2005)
 19. Radiological monitoring around Krško, Nuclear Power Plant Krško, Slovenija, Stipe Lulić
 20. Morinje Bay ecological study. Goran Mihelčić
 21. Ecotoxic metals in aquatic organisms in NP "Plitvička jezera", Dario Omanović
 22. Assessment of selected POPS in the atmosphere and water ecosystems from waste materials generated by warfare in the area of former Yugoslavia, Mladen Picer
 23. Nano-systems and nano-tecnology: The role of enzymes in the formation of inorganic colloids, Ivan Sondi (Croatia-Slovenia Collaboration Project)
 24. Smart Particle Analyzer, Vesna Svetličić and Vera Žutić (STP Pilot project, World Bank and MZOS)
 25. Sava River Basin: Sustainable Use, Management and Protection of Resources, Biserka Raspor (EU FP6-2002-INCO-WBC-1)
 26. Development of Information Systems for the Management of Fairways on Drava and Danube Rivers, Ivica Ružić i Jadranka Pečar-Ilić (Ministry of the Sea, Tourism, Transport and Development, Directorate for Inland Navigation, Zagreb, Croatia)
 27. Development of an international standard of data warehouse for Danube waterway, Ministry of sea, tourism, transport and development. Ivica Ružić (INTERREG III B CADSES cooperation)
 28. Strategic Environmental impact assessment study of fish and shellfish culture in Krka estuary, Emin Teskeredžić
 29. Environmental impact assessment study of fish and shellfish culture in Kaldonta bay, Island Lošinj, Emin Teskeredžić
 30. Development of new type of electrochemical sensor and measurement system for reactive microparticles, Vera Žutić, (HITRA)
 31. Mechanism of mucilage formation in the Northern Adriatic Sea, Vera Žutić (Bilateral Cooperation project with NSF, USA, Scripps Institution of Oceanography, UCSD)

EDUCATIONAL ACTIVITIES

Oceanography

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

Environmental protection and nature conservation

Since 2001 an interdisciplinary M.Sc. study in cooperation with the University J.J. Strossmayer, Osijek. During 2005 the study has been upgraded to the Ph.D. level. B. Ćosović.

Environmental management

(an international study)

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

Ph.D. thesis

Begonja Kolar A., Biphenyl-degrading microbial communities as potential catalysts for aerobic degradation of polychlorinated biphenyls in marine environment. Faculty of Food Technology and Biotechnology, University of Zagreb, December 2005.

BOOKS

1. Hackenberger B. K. and Legović T. Alexandrina Statistica, CD, Natura Aeterna, Osijek, 2005.
2. Raspor B., Guest editor, Croatian Waters **53** (2005), a collection of 20 reviewed professional papers presented at the 9th Meeting of Laboratories accredited for water quality determination, Vinkovci, 7-10-6-2005 (in Croatian).



Figure 3: Lecture notes and a collection of statistical freeware for environmental science.

AWARD

Pečar-Ilić J., Ružić I. Application of GIS and Web technologies for Danube waterway data management in Croatia. The best scientific paper in application of GIS, EnviroInfo, Brno, 2005.



Figure 4: A comparison of the digital map of Drava River within ETRS-89 geodetic system and the Landsat 7 satellite picture.

SELECTED PUBLICATIONS

1. Ahel M, Tepić N, Terzić S. Spatial and temporal variability of carbohydrates in the northern Adriatic – A possible link to mucilage events. *Sci Tot Environ* 2005: 353: 139.
2. Ciglencečki I, Krznarić D, Helz G R. Voltammetry of copper sulphide particles and nanoparticles; Investigation of the cluster hypothesis. *Environ Sci Tech* 2005: 39: 7492.
3. Cuculić V, Pižeta I, Branica M. Voltammetric determination of stability constants of iron(III) - glycine complexes in water solution. *J Electroanal Chem* 2005: 583: 140.
4. Ćosović B. Surface-active properties of the sea surface microlayer and consequences for pollution in the Mediterranean Sea. In: *The Mediterranean Sea, Handbook of Environmental Chemistry* (Salot A ed.). Springer-Verlag, Berlin Heidelberg, 2005: 15: 269.
5. Dragun Z, Raspor B. Direct determination of Cd in NaCl containing metallothionein

- fractions of different red mullet tissues by GF-AAS. *J Anal At Spectrom* 2005: 20: 1121.
6. Erk M, Ruus A, Ingebrigsten K, Hylland K. Cadmium accumulation and Cd-binding proteins in marine invertebrates-A radiotracer study. *Chemosphere* 2005: 61: 1651.
 7. Garnier C, Pižeta I, Mounier S, Cuculić V, Benaim J Y. An analysis of distinguishing composite dissolved metal-ligand systems measurable by stripping voltammetry. *Anal Chim Acta* 2005: 538: 263.
 8. Gašparović B, Plavšić M, Čosović B, Reigstad M. Organic matter characterization and fate in the subarctic Norwegian fjords during late spring/summer period. *Estuarine Coastal and Shelf Science* 2005: 62: 95.
 9. Giani M, Savelli F, Berto D, Zangrando V, Čosović B, Vojvodić V. Temporal dynamic of dissolved and particulate organic carbon in the northern Adriatic Sea. *Sci Total Env* 2005: 353: 126.
 10. Goodwin A, Lawrence A, Banks C, Wantz F, Omanović D, Komorsky-Lovrić Š, Compton R. On-site monitoring of trace levels of free manganese in sea water via sono-electroanalysis using a boron-doped diamond electrode. *Anal Chim Acta* 2005: 533: 141.
 11. Grahek Ž, Rožmarić Mačefat M. Determination of radioactive strontium in seawater. *Anal Chim Acta* 2005: 534: 271.
 12. Ivanković D, Pavičić J, Erk M, Filipović Marijić V, Raspor B. Evaluation of the *Mytilus galloprovincialis* Lmk. digestive gland metallothionein as a biomarker in a long-term field study: seasonal and spatial variability. *Mar. Pollut. Bull.* 2005: 50: 1303.
 13. Janeković I, Kuzmić M. Numerical simulation of the Adriatic Sea principal tidal constituents. *Annales Geophysicae* 2005: 23: 3207.
 14. Kozarac Z, Risović D, Frka S, Möbius D. Reflection of light from the air/water interface covered with sea-surface microlayers. *Marine Chemistry* 2005: 96: 99.
 15. Krznarić D, Ciglenečki-Jušić I. Electrochemical processes of sulphide in NaCl electrolyte solutions on mercury electrode. *Electroanalysis* 2005: 17: 1317.
 16. Obhodaš J, Vdović N, Valković V. Dynamics of soil parameters relevant for humanitarian demining. *Nucl Instr and Meth in Phys Res B.* 2005: 241: 759.
 17. Pižeta I, Billon G, Omanović D, Cuculić V, Garnier C, Fischer, J C. Pseudopolarography of lead (II) in sediment and in interstitial water measured with a solid microelectrode. *Anal Chim Acta* 2005: 551: 65.
 18. Rožić M, Cerjan-Stefanović Š, Kurajica S, Rožmarić Mačefat M, Margeta K, Farkaš A. Decatination and dealumination of clinoptilolite tuff and ammonium exchange on acid-modified tuff. *J Colloid Interface Sci* 2005: 284: 48.
 19. Rožić M, Rožmarić Mačefat M, Oreščanin V. Elemental analysis of ashes of office papers by EDXRF spectrometry. *Nucl Instr Meth Phys Res B* 2005: 229: 117.
 20. Sondi I, Salopek-Sondi B. The influence of the primary structures of urease enzyme on the formation of CaCO₃ polymorphs: A comparison of plant (*Canavalia ensiformis*) and bacterial (*Bacillus pasteurii*) ureases. *Langmuir* 2005: 21: 8876.
 21. Suber L, Sondi I, Matijević E, Goia D V. Preparation and the mechanisms of formation of silver particles of different morphologies in homogeneous solutions. *J Colloid Interface Sci.* 2005: 288: 489.
 22. Svetličić V, Žutić V, Hozić Zimmermann A. Biophysical Scenario of Giant Gel Formation in the Northern Adriatic Sea, *Ann. NY Acad. Sci.* 2005: 1048: 524.
 23. Zelić M. The Influence of Rhodium(+3) on Voltammetry of Selenium(+4) in Perchloric Acid. *Electroanalysis* 2005: 17: 1302.

Center for Marine Research



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

CIM

DEPARTMENT ORGANISATION

Head: Nenad Smodlaka

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

- ⇒ Laboratory for ecology and systematics, Ana Travizi
 - ⇒ Laboratory for processes in the marine ecosystem, Danilo Degobbi
 - ⇒ Laboratory for marine molecular toxicology, Renato Batel
 - ⇒ Laboratory for ecotoxicology, Bartolo Ozretić
3. Ecophysiological studies and stress response in marine organisms, Čedomil Lucu
 4. Systematic research of the Adriatic Sea as a base for sustainable development of the Republic of Croatia (Project «Adriatic»), Croatian national monitoring programme, Nenad Smodlaka

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

1. Mechanism of long-term changes in the Adriatic Sea ecosystem, Danilo Degobbi
Programmed biosynthesis and genotoxic risk assessments, Renato Batel
2. Physiological and biochemical indicators of toxicological stress in marine biota, Bartolo Ozretić

Center for Informatics and Computing



<http://www.irb.hr/cir>

CIR

ORGANISATION OF THE CENTER

Head: Karolj Skala

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

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

OVERVIEW OF THE CENTER

Scientific Research and Development

CIR successfully finalised scientific work on the detection of non-stationary sources and distributed information processing. CIR continues the eScience program based on ICST (Information Communication Science Technology) on Grid platforms, concerning the realisation of the National Grid Initiative poly-project CRO-GRID with 11 institutions and over 50 explorers. The goal of the project is to establish a national computing grid, and is presently in a very advanced

phase. CIC is the leader of the CRO-GRID Applications project and member of the CRO-GRID Infrastructure project. CIR is also developing a Grid Portal through which scientists will be able to access the grid computing resources and submit complex compute-intensive jobs.

A further important realisation of CIR in 2005 was successful development work on the EU FP6 project SEE-GRID. We organised the meeting of project reviewers after the first project year in Opatija, getting a high reviewers mark for the whole project. CIR successfully submitted the application as a member of the Croatian Joint Research Unit to become established as a permanent participant in the EU F6 EGEE II e-Science programme. CIC established a collaborative contract with CERN enabling one of our young assistants to become an associated member of the grid project at CERN.

We organised the First Virtual Grid Christmas Party between RBI and CERN using our new teleconferencing facilities.

At the end of the year we started with the Scientific Visualisation Programme. The new Grid paradigm in sciences imposes new great possibilities of processing huge quantities of natural (measured) or generated (simulated) data. The processing is conducted in an organized infrastructure

with access through the Grid portal to clusters of computers. Systematic and well-established continuous scientific research is initiated in several vital areas of the field; scientific visualization methods are set up in the areas where biggest scientific activity is present, i.e. in the area of complex problem solving by using distributed processing systems. This causes new focused development, which changes scientific and technical intelligence, resulting in pragmatic changes in the area of data processing and visualization by introducing methodologies for everyday practical application in relevant scientific disciplines.

The research aim within the eScience programme is to contribute to and upgrade the contemporary scientific work technology with advanced methods, procedures and new representation of complex data with a certain degree of interaction in parallel and distributed processing environments.

Successful reimplementation and parallelisation the random forests algorithm (PARF) was done. The random forests algorithm is one of the best among known classification algorithms, able to classify large quantities of data with great accuracy. The original algorithm is adapted to structured programming language Fortran 90. PARF's source code can be found at <http://parf.irb.hr>.

Remote IR temperature measurement through the web (ThermoWEB) was developed, using a NEC Thermo tracer TH7102WL camera with full control and remote functionality. The result is an improved remote thermovision system using web communication protocols.

PARF and ThermoWeb were both developed with the financial support of the Ministry of Science, Technology and Sports of the Republic of Croatia.



Figure 1: The CIR eScience both at the MIPRO conference

INFORMATION SYSTEMS DEVELOPMENT AND SERVICES

New improvements that CIC implemented in the RBI information infrastructure in 2005 are Milter and Greylisting on the mail server, load balancing and failover of the DHCP server, NetDISCO for network maintenance, OTRS ticketing system for end users and Bacula backup system for servers. All of these innovations are open source software that is modified to meet our needs.

Milter is a module for Sendmail that has an Application Programming Interface (API) so that programmers can add their own, new functionality to mail processing. In addition to it, MIMEDefand is also installed, a framework that uses Milter API for e-mail filtering. On top of that Greylisting uses this framework to process e-mails during the process of delivery to our system. Greylisting is a new method of blocking significant amount of spam at the Mail server level, but without resorting to heavyweight statistical analysis or other heuristic approaches. This package of tools sped up our Mail server by 50 percent.

The DHCP server is a very important service because it provides IP addresses to many clients on RBI's network. To avoid sin-

gle point of failure we implemented failover functionality on our two DHCP servers, as well as load balancing, so clients can always get their IP addresses due to redundant server services.

NetDISCO is a network maintenance package that has a web interface, so that all network administrators can use a common internet browser and see what is happening on the network from wherever they are.

The OTRS ticketing system for end users is an upgrade of the existing OTRS system for administrators and helpdesk employees. This new system allows every single user to add new tickets (their problems) to system, see the status of their ticket, the person responsible for their ticket, as well as other useful information about their tickets (problems).

The Bacula backup system is installed on a backup server as well as on all servers that are maintained by IS department. This system is an automated backup system that makes backups of all servers incrementally. All backups are performed using hard disks, so the data recovery is very fast and reliable.

The web CMS system entered the second year of usage and continues to function without any major problems with steady usage increase in all major categories (bandwidth, unique visitors, number of visits etc.)

The Services department continued to offer its service activities, i.e. printing and plotting for the needs of the whole of RBI, which has become a standard and much appreciated service for many RBI employees. The printing/plotting service offers colour poster printing as well as many forms of A4 and A3 colour or B/W printing.

By the end of 2005, full blown teleconferencing services were introduced by the adaptation of an existing lecture room into a

TCR (TeleConference Room), both in terms of acquiring professional TCR equipment and proceeding with necessary construction works.



Figure 2: Teleconferencing IRB-CERN, Virtual Christmas Party

TOP ACHIEVEMENTS OR HIGHLIGHTS IN 2005

Development of new technology and software

- Established Grid Cluster node in EGEE environment.
- Excellent results after the first year of SEE GRID EU FP6 project.
- Debian Cluster Components, a Linux Cluster Distribution was finalized as Open-Source, and is available on <http://dcc.irb.hr/>. Additionally DCC/Live, a 'Cluster on a CD' was developed for educational and research purposes.
- Parallel Random Forest Algorithm, available on <http://www.parf.irb.hr>.

Infrastructure support improvements

- Within the framework of CRO-GRID, a new Network Storage System was installed.
- Installation of TCR equipment and implementation new teleconferencing services.

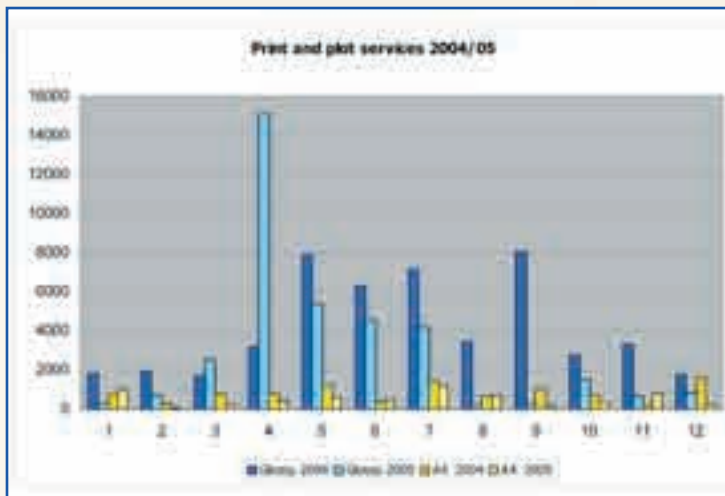


Figure 3: Web server statistics

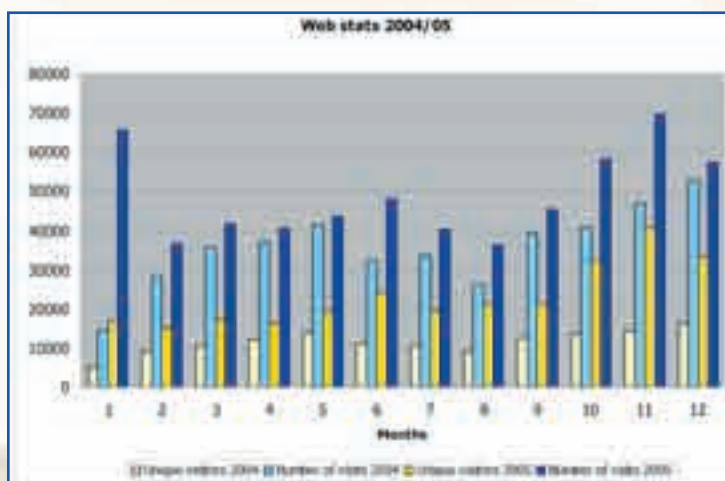


Figure 4: Summary of print and plot. Glossy paper plot length and A4 printed pages total

Project initiatives

CIR submitted 3 new EU F6 project proposals inside the ICT, LIFE and INCO programmes.

- Mobile Broadband Wireless Network for Grid Services, MOBiWaN, FET Project proposal.
- Forest Fire Monitoring on Ecological Grid, LIFE Third Countries 2005.
- Centre for Scientific visualisation, FP6-2005-INCO-WBC/SSA-3, project proposal.

EDUCATIONAL ACTIVITIES

- The Centre provides 4 undergraduate and 3 graduate courses at Faculty of Electrical Engineering and computing and Faculty of Graphical Arts at the University of Zagreb.
- Attendance at the International Grid Summer School on Grid Computing, Budapest, Hungary.
- Workshop on Parallel Programming and Cluster Computing, MIPRO Opatija.
- System on chip, hands-on workshop, RBI, Zagreb.
- PADS electronic Design, teleconferencing workshop eCAD, RBI Zagreb.
- As a Grid dissemination activity, CIC started the "GridVision" initiative (<http://gridvision.irb.hr/>), and produced the first "GridVision" promotional film, downloadable at <http://www.irb.hr/en/cir/gridvision/>. The "GridVision" initiative was very well received by the EGEE II consortium and its further development is planned inside EGEE II NA3.

ORGANISATION OF CONFERENCES AND SPORTING EVENTS

CIR organized the annual Conference Hypermedia and Grid Systems as part of the International Convention MIPRO in Opatija, and a traditional yearly gathering of the sailors from Universities and scientific institutes at the University Sailing Regatta in Zadar.

SCOPE OF THE PROJECTS

Applied scientific project

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

Technological projects

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

Information technology projects

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

International projects

1. COST#276 Information and Knowledge Management for Integrated Media Communication, national coordinator, Karolj Skala.
2. Grid enabled Infrastructure Development, SEE-GRID, EU FP6, con. no. 002356, Karolj Skala.
3. SEE-GRID-2, EU FP6, Karolj Skala
4. eScience project EGEE II, EU FP6, JRU member coordinator Karolj Skala.
5. Inter institutional testbed for e-Science applications, Jožef Štefan Institute, Ljubljana CRO-SLO bilateral project, Karolj Skala.
6. Parallel Application Development on Grid, SZTAKI, Budapest, HUN-CRO bilateral project, Karolj Skala.
7. Debian LCG porting, Svannah project, CERN.

Other Internal self-financing IT projects

1. Enhancements of the internal WLAN (wireless computer network).
2. Server park improvement.
3. Development of Cluster computing resources.
4. LDAP data base implementation.
5. Server monitoring system improvement.
6. Development DHCP and NAT services.
7. New mail server improvement.
8. Storage Area Network implementation.

SOFTWARE PRODUCTS

- PARF, Parallel Random Forest Algorithm, <http://www.parf.irb.hr/>.
- ThermoWeb, Remote control and temperature measurement over WEB, <http://www.irb.hr/hr/cir/projects/info/thermoweb/>.
- DCC Live and Debian Cluster Components, Linux Cluster Distribution software package announced as an Open-Source product, and is available on <http://dcc.irb.hr/>.

CONTRACT BASED COLLABORATION WITH OTHER INSTITUTIONS

- Institute for Software Science of the University of Vienna, Austria.
- CERN-RBI collaboration contract.
- Jožef Štefan Institute, Ljubljana, Slovenia
- Hungarian Academy of Science Institute SZTAKI, Budapest, Hungary.
- Contract for collaboration in the field of GRID technology, Ericsson - Nikola Tesla, Zagreb.
- Memorandum of Joint ICT development, SRCE, Zagreb.

- EU F6 Consortium members SEE-GRID
- CRO-GRID Consortium member.
- EU F6, EGEE II JRU Consortium member.
- Mentor Graphics/Wedasoftware, Vienna, Austria.

SELECTED PUBLICATIONS

1. Skala K, Šojat Z. Image Programming for Scientific Visualization by Cluster Computing. ICAS/ICNS, Tahiti, 2005, 93-97.
2. Skala K, Pavković N, Šojat, Z. Parallel Programming and Scientific Visualization Applications, 8th COST 276 Workshop, NTNU Trondheim, Norway, May 26 - 28, 2005, 99-102.
3. Topić G, Šmuc T, Šojat Z, Skala K. Reimplementation of the Random Forest Algorithm in Parallel Numerics, Theory and Applications, Vajtersic, Marian et al. (eds). Salzburg : University of Salzburg, 2005. 119-128.
4. Pavković N, Skala K, Vidić V, Šojat Z. Bioinformatics Application Oriented IT Deployment Model in Parallel Numerics, Theory and Application, Vajtesic, Marian et al. (eds). Salzburg : University of Salzburg Austria, 2005. 217-222.

Center for Nuclear Magnetic Resonance



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

Head: Dražen Vikić-Topić until July 21st
Replacement: Željko Marinić

OVERVIEW OF THE CENTRE

The Centre for Nuclear Magnetic Resonance (NMR), the only academic NMR facility in Croatia, was founded in November 2003 as an independent unit of the Ruđer Bošković Institute. The Centre performs scientific research and scientific services as well as providing educational and professional support for the scientists and researchers of the Ruđer Bošković Institute (RBI). In addition, similar support is given to scientists and students from the Universities of Zagreb, Rijeka, Split and Osijek, as well as to scientists and researchers from governmental institutions and the pharmaceutical industry. Research work at the NMR Centre includes different topics in organic, inorganic, bioorganic, pharmaceutical chemistry and biotechnology. Theoretical calculations of molecular structures and NMR spectral parameters are carried out in order to support the experimental measurements. Investigations of natural compounds and photochemistry products are also in progress. The Centre is also involved in undergraduate and graduate studies at

the Universities of Zagreb and Osijek. The Centre's equipment at RBI includes Bruker Avance 300 and 600 MHz NMR spectrometers, purchased in 2002. The subsidiary of NMR Centre, located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb, is using a Varian Gemini 300 MHz NMR spectrometer.

TOP ACHIEVEMENTS

To optimize the use of expensive physical measurements, first the properties of model molecules were calculated using sophisticated quantum mechanical approaches. Measurement methodology optimized for the target molecules was developed and implemented on the NMR spectrometers. Based on the results from the previous steps, the structure of a phosphorous-containing bacterial carbohydrate was determined.

NMR and IR spectroscopic investigations of interactions of pharmaceutically active molecules were carried out as well. In this respect, the antimicrobial peptides are of interest since, in some cases, small fragments can mimic and even supersede the activity of the whole molecule. The structure, bioactivity and sense anti-sense interactions of short peptide fragments, with five to thirteen amino acids, were investigated.

INVITED LECTURES AT INTERNATIONAL CONFERENCES

1. Smrečki V. Theoretical Simulation of Conformational Influence on NMR Chemical Shielding Anisotropy. 14th International Symposium "Spectroscopy in Theory and Practice", Nova Gorica Polytechnic, Nova Gorica, Slovenia, 2005

ORGANIZATION OF INTERNATIONAL CONFERENCES AND COURSES

1. The 20th Dubrovnik International Course & Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Dubrovnik (IUC), July 20-25, 2005

PROJECTS

Projects supported by the Ministry of Science, Education and Sports (MZOŠ) and collaborative projects

1. Nuclear Magnetic Resonance and Calculations of Bioorganic Molecules, Dražen Vikić-Topić (MZOŠ)
2. Spectroscopic and Quantum Chemical Study of Models for Biomolecular Interactions, Vilko Smrečki (bilateral collaboration with Austria)

Contracts with industry

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

International collaborations

1. Nenad Juranić, Mayo Clinic and Foundation, Rochester, MN, USA
2. Norbert Mueller, Institute of Chemistry, Johannes Kepler University, Linz, Austria
3. Ljupče Pejov, Faculty of Natural Sciences and Mathematics, Skopje, Republic of Macedonia
4. Janez Plavec, National Institute of Chemistry, Hajdrihova 19, Ljubljana, Slovenia
5. Nicolay Sergeevyev, Department of Chemistry,

Moscow State University, Moscow, Russia

6. Vladimir Sklenar, Faculty of Science, Masaryk University, Brno, The Czech Republic



Figure 1. The NMR operators room with a view on a 7T magnet (300 MHz frequency for ^1H NMR)



Figure 2. The instrumental room with a 14T magnet (600 MHz frequency for ^1H NMR)

TEACHING

1. Chemical Toxicology: School of Health Studies, University of Zagreb, Dražen Vikić-Topić
2. Spectroscopic Methods in Structural Analysis: Graduate Studies in Analytical Chemistry, Faculty of Science, University of Zagreb, Dražen Vikić-Topić
3. Application of NMR Spectroscopy in Determination of Structure and Dynamics of Organic and Bioorganic Molecules: Graduate Studies in Organic Chemistry, Faculty of Science, University of Zagreb, Dražen Vikić-

4. Modeling of Protein Structure and Function - Applications in Biomedicine: Graduate Studies at School of Medicine, University of Zagreb, Dražen Vikić-Topić
5. Spectroscopic Methods: Graduate Studies in Environmental Protection, University of Osijek, Dražen Vikić-Topić

SELECTED PUBLICATIONS

1. Diudea MV, Nagy CL, Silaghi-Dumitrescu I, Graovac A, Janežić D, Vikić-Topić D. Periodic Cages. J Chem Inf Model 2005: 45: 293.
2. Sychrovsky V, Mueller N, Schneider B, Smrečki V, Špirko V, Šponer J, Trantirek L. Sugar Pucker Modulates the Cross-Correlated Relaxation Rates across the Glycosidic Bond in DNA. J Am Chem Soc 2005: 127: 14663.
3. Škorić I, Basarić N, Marinić Ž, Višnjevac A, Kojić-Prodić B, Šindler-Kulyk M. Synthesis and photochemistry of b, b'-di(2-furyl) substituted o-divinylbenzenes. Intra- and/or intermolecular cycloaddition as an effect of

4. Steindl C, Schäffer C, Smrečki V, Messner P, Müller N. The secondary cell wall polymer of *Geobacillus tepidamans* GS5-97(T): structure of different glycoforms. Carbohydr Res 2005: 340: 2290.
5. Tješić Drinković Du, Tješić Drinković Do, Štambuk N, Konjevoda P, Votava Raić A, Vinković M, Vikić-Topić D. Alpha-melanocyte stimulating hormone reduces colonic damage in rat model of inflammatory bowel disease. Croat Chem Acta 2005: 78: 535.



Figure 1: The building of the NMR Centre



Library



<http://library.irb.hr>

Head of Library: Jadranka Stojanovski

OVERVIEW OF LIBRARY ACTIVITIES

In 2005 RBI Library remains focused on its mission to support the research and educational activities of the RBI scientific community. The Library provided reliable access to scientific content in print and electronic format, ensuring that the selection, acquisition, cataloguing, storage and preservation of scholarly information is according present requirements and needs.

Goals and Priorities

The RBI Library continues to innovate with information technology not only at RBI, but also in the larger context of the Croatian academic and research community. The Library continues to exist both as a physical and an online entity. In 2005 the average number of visits of our library web site is more than 3000 daily.

The way in which scholarly information is published and made accessible is changing constantly and Library tried to respond to these changes. Nationally and internationally digital repositories are beginning to change the way the results of the scholarly activity reach scientists and researchers. Promotion and development of and institutional online

repository for Ruđer Bošković Institute is a clear priority for the Library. Two leading programmes for digital repositories, EPrints and DSpace were installed and preliminary testing had been undertaken in order to follow the new demands of storing and preserving digital content for archival timeframes. One of our goals is to make our digital document repositories interoperable with other emerging technologies and work practices.

The Library is working hard to maintain the stability and reliability of its hardware and software, and to provide continuing education and training for the Library staff in a range of information technology tools and topics. One of the greatest ongoing challenge is finding the balance between supporting local initiatives and the larger centralized projects on national level, encouraging creativity throughout our system without compromising support to the many existing services.

Library collections

The Library's book collection amounts to some 34000 volumes, 300 of which were newly acquired in 2005. E-books were acquired and added to the collection through the Centre for online databases (42 e-books). The journal acquisition model for 2005 was simpler then previous years and turned toward big publish-

ers. This resulted in some discontinuity in subscription for some very important titles published by smaller publishers. 11230 e-journal titles were purchased by the Ministry of Science, Education and Sport (MSES) via consortia agreements with major scientific publishers (Springer & Kluwer 1328, Wiley 220, EBSCO 6800, Elsevier 1750, Oxford University Press 180, Cambridge University Press 135, Blackwell 817), and 9360 e-journal titles were available free of charge and accessible through EJOL (Electronic Journal Online Library at <http://ejol.irb.hr>) and EZB (Elektronische Zeitschriften-bibliothek at <http://rzblx1.uni-regensburg.de/ezeit/>). The access to the relevant bibliographic and full-text databases was provided through the Centre for online databases (<http://www.online-baze.hr>), maintained by the RBI Library in cooperation with the Croatian Academic and Research Network CARNet for the academic and research community in Croatia. The RBI Library has a well-established interlibrary loan service with Croatian and foreign libraries. In 2005 it fulfilled 1066 requests for documents made by members of the RBI, and over 1145 requests from other libraries.

Computing Infrastructure

The RBI Library has this year acquired two new Dell servers with the support of the Ministry of Science, Education and Sport. As the most visible part of RBI, the Library's computer systems are continually under threat from network intruders, and we must also uphold increasingly complex rules about access control and security for the networked digital material we license for

RBI. The connection between good network security and user convenience continues to be a challenging and time-consuming task. Together with existing computing equipment, the Library's computing infrastructure consists of following:

- DELL PowerEdge 2800 #1
(Debian GNU Linux)
- DELL PowerEdge 2800 #2
(Debian GNU Linux)
- DELL PowerEdge 1500sc
(FreeBSD)
- SUN ENTERPRISE 250
(Solaris 7)
- SUNFire 280R
(Solaris 7)
- SUNFire V880
(Solaris 8)
- PC (AMD700)
(FreeBSD)
- PC (AMD700)
(Debian GNU Linux)
- 13 personal computers for Library staff and 5 personal computers for Library patrons

Ongoing services

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 library staff assistance to be given indirectly. This assistance included:

- PRESKOK – federated search of the Croatian academic and research libraries online catalogues (<http://preskok.irb.hr>)
- Union online catalogue for sciences - 27 libraries included (<http://prirodo.irb.hr>)
- SEND - Interlibrary Loan service (<http://send.irb.hr>)
- CROSBI – Croatian Scientific Bibliography (<http://crosbi.szi.hr>)
- Who's Who in Croatian Science (<http://tkojetko.irb.hr>)
- CMS for web academic and research libraries (<http://knjiznice.szi.hr>)
- RBI Annual Report site (<https://godisnji-izvjestaj.irb.hr/public/>)
- Centre for online databases (<http://www.online-baze.hr>).

TOP ACHIEVEMENTS

HRČAK

Together with University Computing Centre SRCE (project leader) and Croatian Information and Documentation Association, we were working on the central portal of Croatian scholarly journals. HRČAK offers access to journals following the Open Access



Initiative (OAI) and supports harvesting of the metadata according to the Metadata Harvesting Protocol (MHP).

CENTRE FOR ONLINE DATABASES

In cooperation with the Croatian Academic and Research Network CARNet we are working on the project Centre for online databases for ten years now trying to provide Croatian academic and research community with the access to the most important online databases and e-journal collections. In 2005 the complete redesign of the web site was done in order to provide more transparent access to all available resources.



SELECTED LECTURES

- Mayer, M.; Vodopijevac, A. SEND - ILL service online. 9th IFLA Interlending and Document Supply (ILDS) International Conference; September 20-23, 2005, Tallinn, Estonia.
- Stojanovski, J.; Melinščak Zlodi, I. Roadmap to Open Access in Croatia. 11th Biennial Conference of the European Association of Aquatic Sciences Libraries and Information Centres; May 4-6, 2005, Split, Croatia.

- Stojanovski, J.; Škvarč, G. Open access initiatives in Croatia. CUC 2005: Meeting users needs - How to fulfill users needs; November 21-23, 2005, Zagreb, Croatia.
- Stojanovski, Jadranka. Scientific information on demand - the Croatian experience. Arbeitsgemeinschaft für medizinisches Bibliothekswesen (AGMB); September 26-28, 2005, Graz, Austria.

SELECTED PUBLICATIONS

- Erman, D. Knjižnica centra za istraživanje mora. *Kemija u industriji*, 54 (2005) 1; 20-21.
- Konjević, S. EURASLIC 11 : Open Waters - Open Sources. *Kemija u industriji*. 54 (2005) 10; 430.
- Pažur, I. Access to electronic journals in the Croatian libraries. Master Thesis. University of Zagreb ; Zagreb, 2005.
- Pažur, I. "From our libraries" yes or no? *Kemija u industriji*, 54 (2005) 3; 157-158.



CONFERENCE ORGANIZATION

- 11th Biennial Conference of the European Association of Aquatic Science Libraries and Information Centres (EURASLIC 11): «Open Waters – Open Sources», Split, Croatia, 4-6 May, 2005.

RUĐER BOŠKOVIĆ INSTITUTE LIBRARY COLLOQUIA

In 2005 we continue to organize popular and well visited RBI Library Colloquia. Through regular monthly lectures and presentations we hosted librarians and information specialists from different academic, special and public libraries, as scientists and teachers from RBI and other institutions to share their experiences with others. The most interesting topics from the field of information sciences were included:

14 December 2005., *dr. sc. Branko Šantić* (Ruđer Bošković Institute, Zagreb): Authors and co-authors of the scholarly articles.

24 October 2005., *Bruce Rosenblum* (Inera Incorporated): Quality Management for Electronic Journal Production and Archiving (PDF).

5 October 2005., *dr. sc. Jelka Petrak* (Central Medical Library, Zagreb) i *mr. sc. Jadranka Stojanovski* (Ruđer Bošković Institute Library, Zagreb): Subject portal for scientific information – challenge for cooperation.

29 June 2005., *Jasna Tingle*, CARNet: E-learning and what can we do with it in Croatia.

27 May 2005., *Richard E. Stern*, Seton Hall University Libraries, SAD: Scholarship in the Promotion & Tenure Review Process: Challenges for Librarians as Applicants & Reviewers.

27 April 2005., *Daniel Glavan, Biblos*, Zagreb: Literary work of Josip Ruđer Bošković.

22 March 2005., *prof. dr. sc. Tatjana Aparac-Jelušić*, Department for information sciences, Faculty of philosophy, University J. J. Strossmayer, Osijek: Academic education of the information specialists and Bologna process.

23 February 2005., *Sandra Čar*, European Documentation Centre, Zagreb: Government publications and other information resources about EU.

INFORMATION TECHNOLOGY

PROJECTS

1. Croatian Scientific Bibliography CROSBİ, Jadranka Stojanovski
3. Centre for online databases, Jadranka Stojanovski
4. Who's Who in Science in Croatia, Jadranka Stojanovski











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