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Ruđer Bošković Institute

Annual Report 2008

Ruđer Bošković Institute

Annual Report 2008



Zagreb, 2009.

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Dear reader,

Welcome to the 2008 Annual Report of the Ruđer Bošković Institute. The report is designed to provide an overview of the most important activities and achievements of Institute's Laboratories and Divisions during the past year. Due to our position as the largest public research institute in natural sciences, biomedicine, marine research and environmental sciences in the country, funded to a large extent by the Croatian Ministry of Sciences, Education and Sports, our mission is dependent upon the particular needs of our society. Specifically, this involves exemplary performance on three principle fronts: the production of high-quality fundamental research, strong involvement in higher education, and the provision of a leading contribution to the growth of the national economy through production of new technologies based on our intellectual property and expertise.

Based on our desire to continue to fulfil our mission as to the best of our ability, 2008 saw us lay the foundations for a series of positive changes in the future. This included the drafting of a new statute governing the future operation and structure of the Institute. This statute has been approved by both the Scientific Council and the Board of Governors of the Institute and is currently being considered at the ministerial level. We also undertook a systematic evaluation of all 86 of the Institute's laboratories and their leaders. The successful completion of this evaluation by the end of the year places us in an ideal position to enter a new phase of operation at the Institute, fully aware of our strengths, weaknesses, opportunities and threats.

Despite the preparations for potential reorganization, we continued to achieve visible results on all three of the principle fronts mentioned above. Striving for excellence in fundamental research continued strongly during 2008 and the most significant results achieved throughout the year are described in the pages of this report. In addition to the substantial ongoing provision of undergraduate and graduate courses by our scientists at Higher Education Institutions all across the country, 2008 saw us sign additional agreements of cooperation with Institutions in

Zagreb and Šibenik. These agreements are designed to further strengthen our contribution to education in Croatia, particularly in regional centres. We also made several advancements towards consolidating a sustainable infrastructure designed to fully utilize the Institute's intellectual property. Much progress was achieved through the ongoing expansion of Rudjer Innovations Ltd., a company established and wholly owned by the Institute, which has been charged with handling the protection of intellectual property and some commercial aspects of the Institute's work.

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

In closing, I have the pleasant duty to thank the RBI scientific and administrative staff for their honest efforts and enthusiasm as well as their many excellent achievements throughout 2008. To you the readers of this 2008 Annual report I would like to express our sincere thanks for your interest and I would like to invite you to send us your opinions, suggestions for improvement and, by all means, proposals for future collaboration.

A handwritten signature in dark ink, reading "M. Žinić". The signature is fluid and cursive, with a large, sweeping 'Z' at the end.

Prof. Dr. Mladen Žinić
Director General

Introduction

In 2008, the Ruđer Bošković Institute (RBI) continued to build on its ever-expanding and highly important base of international relationships and collaborations. Almost 100 foreign scientists delivered lectures ranging in subject from black holes to river sediments. With each and every lecture came the opportunity to strengthen existing ties or open up new avenues of collaboration between RBI scientists and our colleagues in the international community. While all lectures were important and integral parts of this endeavour, special mention is warranted by the visits of members of our International Scientific Board (ISB). Namely, in May, we were fortunate enough to host Professor Egon Matijević, from Clarkson University in New York, when he delivered a fascinating seminar about colloid aspects of chemical mechanical planarization. Some months later, in September, we were honoured to receive Professor Roberto Peccei, who engaged us with his lecture on matter-antimatter asymmetry in the universe and an arrow for time.

The year of 2008 saw a large number of official delegations visit the Institute. In January, we received His Excellency Mohammad H. Fadaifard, the Iranian Ambassador to Croatia, for discussions on possible collaboration in fundamental research. In April, as part of an information day on the European Commission, the RBI hosted Doctor Roland Schenkel, Director-General of the European Commission's Joint Research Centre. In the same month, we were visited by delegations from the British Embassy and the British Council. In particular, we were pleased to host His Excellency Sir John Ramsden, the British Ambassador to Croatia, Anamarija Jandrasek, from UK Trade and Investment, Adrian Chadwick, the Director of the British

Council in Croatia, and Rosana Besednik, the Arts, Science and Society Manager of the same organization. We also received two visits from dignitaries of the Slovak Republic: in April, the Ambassador of the Slovak Republic to Croatia, His Excellency, Jan Banas, and in September, Mr. Dušan Čaplovič, Deputy Prime Minister of the Government of the Slovak Republic for Knowledge-Based Society, European Affairs, Human Rights and Minorities. A delegation from the Indonesian Embassy in Zagreb, including His Excellency Mangasi Sihombing, the Indonesian Ambassador to Croatia, was hosted at the RBI in April. The month of June saw the visit of a Japanese delegation, including representatives from the Ministry of Education, Culture, Sport, Science and Technology (MEXT), the Japan Science and Technology Agency (JST), the Japan Society for the Promotion of Science (JSPS), and the Japanese Embassy in Zagreb. This visit was followed, in September, by a delegation comprised of representatives of various Japanese companies involved in the nuclear energy sector, including Mr. Toshikazu Hosoda, the president of CHIYODA TECHNOLOGICAL, with whom the RBI has enjoyed a productive collaboration for a number of years now.

In April, we received visits from the German Federal President, Mr Horst Köhler and Dr. Volker Wittwer, the acting director of the Fraunhofer Institute for Solar Energy in Freiburg. Following these visits, a letter of intent concerning collaboration in German and Croatian industrial and research projects in the area of thin-film solar cells envisaged to involve the RBI, the Fraunhofer Institute for Solar Energy, INTERPANE Glas Industrie AG Lauenförde, and the Croatian company Lipik Glas, was signed.

In January, Christopher John Hull, Secretary General of the European Association of Research and Technology Organisations (EARTO), visited the RBI. Subsequently, the Institute became a member of EARTO in 2008. Accordingly, Croatia became a full member of EARTO, while the representative of RBI, Neven Žarković, became a member of the EARTO executive board.

The participation of RBI scientists in European scientific networks remained one of the Institute's top priorities in 2008. For example, in March, we staged an IAEA workshop entitled: "Regional Training Course on How to Write Competitive Research Proposals for Various Funding Programmes". In July, we sent a delegation from RBI to Brussels to present the Institute at a Workshop on Croatian Research and Technological Development hosted by the Croatian Chamber of Economy. In addition to the 13 FP6 projects that are still ongoing at the Institute, 5 FP7 contracts were signed in 2008. Numerous other proposals have been submitted and are awaiting evaluation. RBI scientists also took an active role in Management Committees of COST actions. Krešimir Pavelić, head of the RBI's Division of Molecular Medicine, was appointed in November as a Secretary General of the European Molecular Biology Conference (EMBC) and *ex officio* member of the EMBO Council. Up until November, he was vice-president of the EMBC. Krešimir Pavelić is also member of the EMBC Strategic Working Party, Member of the Standing Committee, European Medical Research Council. Tarzan Legović, head of the Division of Marine and Environmental Research remains the Secretary General of the International Society for Ecological Modelling.

The RBI signed several Memoranda of Understanding in 2008. For example, a contract was signed with the Department of Public Health "Andrija Štampar" concerning scientific and technical cooperation in relation to joint projects in the areas of public health and ecology. In addition, we also signed an agreement

for educational and scientific cooperation with the Australian Research Council's Centre of Excellence for Free Radical Chemistry and Biochemistry. In the area of higher education, agreements were reached with the Agricultural Faculty in Zagreb and the Polytechnic College in Šibenik, while an agreement of business cooperation was signed with the town of Otočac. Finally, a joint agreement on collaboration was signed by RBI, Ruđer Innovations Ltd. and TECNA S.R.L., a diagnostics firm situated in Trieste, Italy.

The RBI's biannual Open Days were held in late April of 2008. Thanks to the dedicated effort of the organizing committee, these days were a great success in displaying the work of the Institute to the general public. Approximately 4200 people passed through the gates over the 3 days of festivities. This included 7 different diplomatic delegations, the Mayor of Zagreb and his entourage, various commercial representatives, members of the media, students and professors from 5 different university faculties and students from 76 schools originating from all over the country. We received very positive feedback from all sides and resounding encouragement to continue with this initiative into the future. Planning is already underway for the 2010 event.

OVERVIEW

The RBI is the largest Croatian research centre for basic sciences, participating also in science applications and higher education. The multidisciplinary character of the Institute is reflected through the different research fields in physics, chemistry, oceanography (including marine and environmental research and geosciences), biology, biomedicine, computer science and electronics/engineering. With an academic staff of 530, including 375 researchers and 155 Ph.D. students, the RBI collaborates worldwide with many research institutions and universities.

The RBI consists of eleven divisions, three centres, a library, as well as sections

for maintenance, technical services and administration. The main bodies of the Institute are the Board of Governors and the Scientific Council, with an important role played by the

International Scientific Board. Their organizational integration with the remainder of the Institute is displayed below (Figure 1).

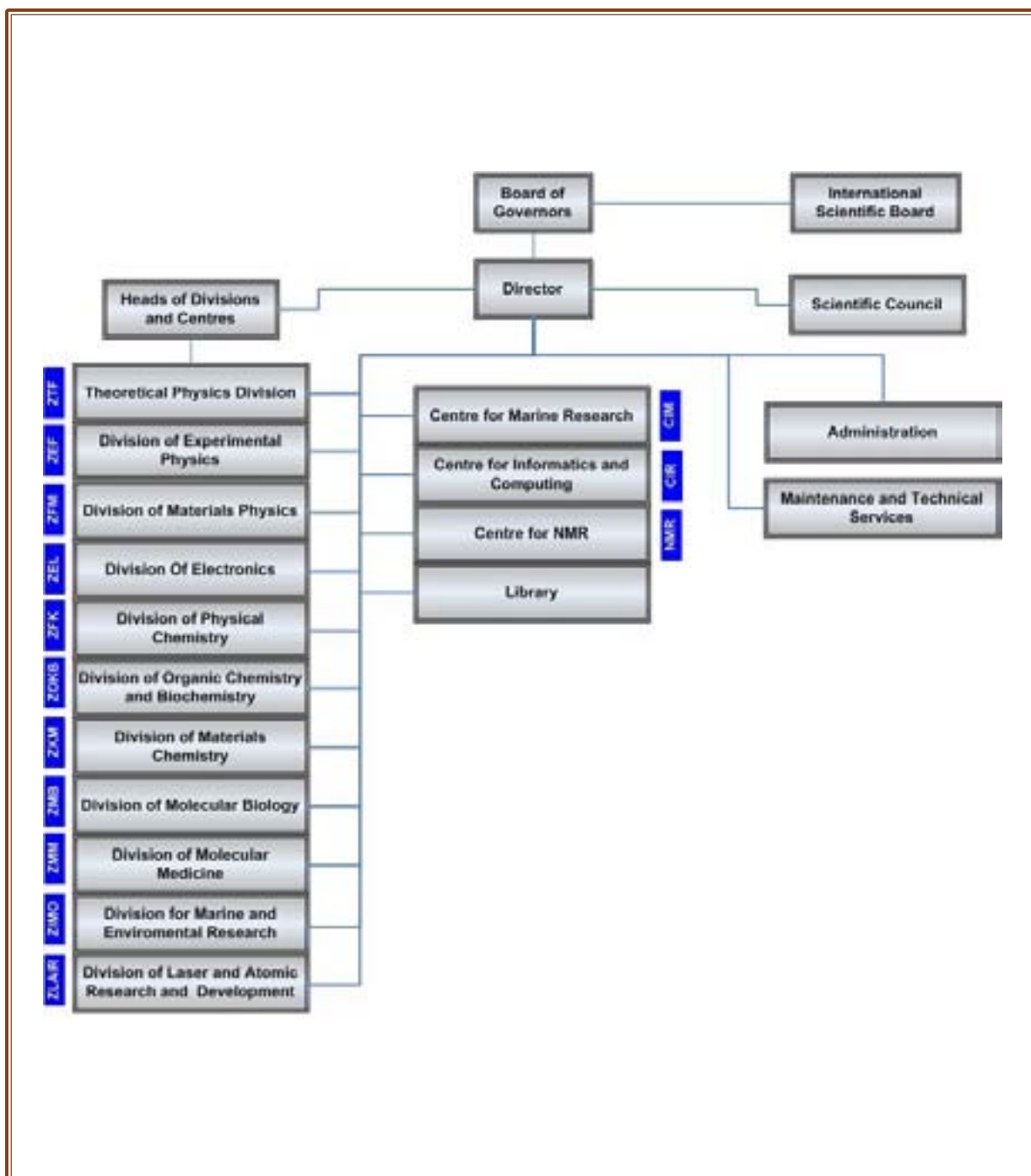


Figure 1. The organizational structure of the RBL.

ORGANIZATION OF THE INSTITUTE

Director: Mladen Žinić

Head of the Scientific Council: Neven Bilić

Chairman of the Board of Governors: Slavko Krajcar

International Scientific Board.

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

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

ACTIVITIES

Fundamental research

The total number of research articles published by RBI scientists in 2008 was 446. Amongst these, 357 were published in journals cited by Current Contents, the majority of which were published in high ranking international Journals. Scientists from the Division of Molecular Medicine authored a monograph on Peripheral Biological Markers in Alcoholism, which was published by Nova Science Publishers in New York, USA. RBI scientists also participated in the editorial process of a further 6 books, 18 book chapters and 2 collections of lecture notes concerning dating techniques.

The details of the many important discoveries made by RBI scientists in 2008 are to be found in the subsequent sections of this report. Nevertheless, we present here a small selection of highlights in order to convey a general impression of the kind of research carried out at the Institute. One breakthrough study, involving scientists from the Divisions of Molecular Biology and Molecular Medicine, was published in the highly cited journal, *Blood*. The research involved gene expression analysis of developmentally important transcription factors from the Ikaros family in

lymphocytes from patients with haematological malignancies, lymphoma, and focused on the differences in the distribution of their messenger RNA (mRNA). Importantly, the results show for the first time that the Aiolos mRNA is overexpressed in primary lymphoma tissues of the non-Hodgkin lymphoma type. On a somewhat different front, scientists working in the Division of Physical Chemistry used molecular modelling techniques to study aspects of the mechanism of Auxin Binding Protein 1 (ABP1), which is a key component of the hormonal regulation of plants. Simulations of the hormone egress from ABP1 revealed three main routes by which an auxin molecule can enter or leave the binding site and the significance of these different pathways was related to the mechanism of action. An illustration describing these results appeared on the front cover of issue 1 of volume 94 of the Biophysical Journal. On the other end of the spectrum, scientists working in the Division of Experimental Physics actively participated in the Crystal Ball collaboration, a new experimental program at the Mainz Microtron facility in Germany. The collaboration is devoted to experiments using energy-tagged photons and among its major goals are the measurements of exotic phenomena such as the anomalous magnetic moment of the Delta resonance, the mass of the eta-meson and double pion production at threshold. In 2008, a paper describing Incoherent Neutral Pion Photoproduction on Carbon 12, co-authored by RBI scientists, appeared in Physical Review Letters, which is one of the most respected and widely read journals in Physics.

Projects

The RBI has 136 projects in basic research, which are funded by the Ministry of Sciences, Education and Sports. In addition, the Institute is involved with 41 international projects (including: 5 FP7, 13 FP6, 6 IAEA, 5 COST, 1 NIH, 3 NATO and 2 INTERREG), as well as 67 applied and technological projects and 4 HITRA projects. This year saw the ex-

pansion of the spectrum of projects offered by the "Unity Through Knowledge Fund", recently introduced by the Croatian Ministry of Sciences, Education and Sports. In addition to the single project contracted from this source in 2007, three new contracts were signed in 2008 and more funding is expected in this vein in 2009. Similarly, collaborative projects with the City of Zagreb were offered for the first time in 2008. One such project has been signed while a further 15 applications are being considered.

An international consortium, including the RBI, was granted a TEMPUS project in 2008. In addition to the RBI, the project, entitled "Opening University towards Society: Linking Education – Research – Innovation", involves 6 Croatian Universities, 6 Foreign Universities, 2 Government Ministries, the City of Zagreb, and 4 additional organizations.

Organization of international conferences

As in previous years, the RBI continued to support the organization of numerous international and domestic conferences. For example, the thirteenth biennial European X-ray Spectrometry Conference was held from 16th to 20th June 2008 in Cavtat. Organized by RBI and co-chaired by Milko Jakšić and Stjepko Fazinić, the conference was attended by 280 scientists from 41 countries and 22 industrial exhibitors. Selected papers were reviewed with regular procedure for publication in the X-Ray Spectrometry journal. Similarly, the 23rd European Congress on Molecular Spectroscopy (EUCMOS-2008) was held in Opatija from the 31st of August to the 5th of September, 2008. Co-chaired by Svetozar Musić and Krešimir Furić, the conference was great success with selected contributions to appear in a special issue of the Journal of Molecular Structure. In May 2008, the Institute jointly with the University of Dubrovnik, hosted for the first time the Annual Reporting Conference of the COST (European Cooperation in scientific and

Technical Research) Domain Committee for Chemistry, Molecular Sciences and Technologies. In November 2008, the RBI organized the conference "Workshop on New Materials in Industry and Medicine: RTD Potential for Collaborative Projects". The conference involved representatives of the partner institutes Jozef Stefan Institute from Slovenia and Joanneum Research Institute from Austria and was organized within the scope of EARTOs Special Interest Group on "Novel bioactive substances for industrial and biomedical use". In September, the 10th Central European NMR Symposium was held at RBI in combination with the 10th Central European Bruker NMR Users Meeting.

Several other equally noteworthy conferences were organized by scientists from the RBI and further information concerning them can be found in the individual reports of the Divisions involved. In addition to their organizational efforts, RBI scientists also participated in many scientific meetings over the year, contributing in the form of invited and accepted lectures as well as numerous poster presentations.

Awards and Recognition

The Croatian Academy of Science and Arts presented its 2008 award for the best publishing achievement to the RBI for its production of "Methods in Molecular Biology", authored by a team of 11 of the Institutes scientists, led by Andreja Ambriović Ristov. Of the many other awards presented to RBI scientists for outstanding achievements in 2008, we have chosen to highlight those earned by the younger members of our staff this year. The RBI and SHIMADZU d.o.o. Zagreb gave the Annual Award of Excellence for the young researchers for the first time in 2008. On this occasion, the award was given to Tomislav Domazet Lošo for his work: A phylostratigraphy approach to uncover the genomic history of major adaptations in metazoan lineages, published in Trends in Genetics in 2007. Marko Košiček received both the Croatian

and International FameLab 2008 awards, organized by the Festival of Science and the British council for the best scientific presentation. David Smith was the 2008 recipient of the Leopold Ružička award for young scientists of the Croatian Chemical Society. Ina Nemet was awarded the Juvenile Diabetes Research Foundation Postdoctoral Fellowship Award (2008-2010). Ana Šarić won the 2007 award for young scientists and artists in the field of neuroscience from the Society of University Teachers, Scholars and Other Scientists - Zagreb. The same organization presented the 2008 award in the field of biology to Branimir Bertoša. Finally, Fran Supek was deservedly selected for the State Award for Science for Ph.D. students in the category of biotechnical sciences.

Education

In 2008, scientists from the Institute contributed in 78 undergraduate courses and 245 graduate courses to the program of higher education in Croatia. Their respective distributions amongst the seven universities at which they were conducted, as well as by the divisions and centres that contributed them are shown in Figures 2, 3, and 4. In addition to the coursework, 22 B.Sc., 6 M.Sc. and 22 Ph.D. theses were completed under the supervision of the RBI academic staff in 2008.

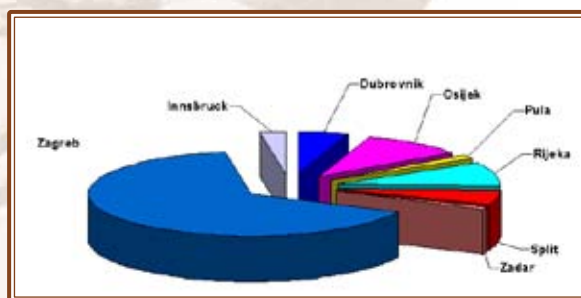
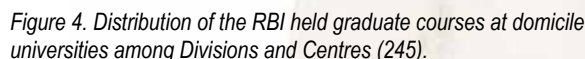
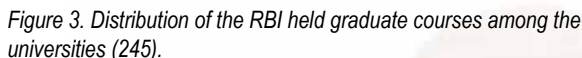


Figure 2. Distribution of the RBI held undergraduate courses among the universities (78).

In 2008, the first 30 students of the graduate studies on Project Management graduated. The study is successfully organized as a joint study of the RBI and the College of



To strengthen the collaboration with regional Universities and increase its contribution in higher education in natural science and biomedicine, the RBI signed agreements of collaboration and partnership with the Agricultural Faculty in Zagreb and the Polytechnic College in Šibenik.

Apart from fundamental research and education, the activities of the RBI also result in various forms of intellectual creations. One important mission of the RBI is the protection

In March, a delegation from RBI and Rudger Innovations Ltd. visited the Finnish Funding Agency for Technology and Innovation, TEKES, in Helsinki.

Rudjer-Medikol Cyclotron Ltd., a spin-off company established by Rudjer Innovations Ltd., continued working towards the reconstruction of the cyclotron facility at RBI. In 2008, all licenses and permits were finalized for the reconstruction and it is expected that the facility will begin producing radioisotopes for use in Positron Emission Tomography in the autumn of 2009.

The new Laboratory for systems biomedicine which includes the Centre for Proteomics and Mass Spectrometry as well as the Centre for Transcriptomics, has been established in 2008. The Centre for Proteomics

and Mass Spectrometry offers commercial services which include amino-acid, protein and peptide sequencing upon isolation and purification. Additionally, the molecular weight analysis could be performed according to the MS and MS/MS measurements. Peptide and protein identification from complex mixtures is performed by using specialized software packages that are directly connected with publicly open databases such as The Protein Data Bank or SwissProt.

A high-pressure liquid chromatography-mass spectrometry (HPLC-MS) instrument (Agilent Technologies) was purchased with the financial help of the Ministry of Sciences, Education and Sports of the Republic of Croatia. The acquisition of the HPLC-MS-MS instrument will contribute to the achievement of the scientific objectives in the majority of chemists at the Institute and open possibilities for introducing new methods and scientific fields.

With the support of the EU FP6 project RBI-AF two quadrupole magnets were added to the existing ion microprobe focusing facility to enable focussing of heavy ion beams, enabling focusing to submicron spot sizes of ions of up to 15 MeV mE/q² rigidity. A laboratory for research in quantum information has been formed for the first time in Croatia. A setup for study of polarization entangled photon pairs was built and used to measure quantum efficiency and single photon timing resolution of a photon detector (constructed in the laboratory).

Revenue and employees

In 2008, the major share of the financial support for the RBI was provided by the

Ministry of Sciences Education and Sports. Compared to 2007, this support increased by 12%. The comparison of the finances over the period 2005-2008 (Table 1) shows a gradual increase. It should be also noted that the revenues originating from international, industrial and service contracts increased by an impressive 84% between 2005 and 2008 although they dropped marginally over the last year. The total number of employees has continued to rise since 2005. However, the recent trend in Ph.D. student numbers, for example, constitutes some cause for concern.

Publication results of fundamental research projects at RBI

Table 2 shows the projects led by RBI scientists which are ranked among the top 15% in the country, according to the Croatian Scientific Bibliography (CROSBI). The number of projects in a particular field of science is taken from the official list of the projects provided by Ministry of Sciences, Education and Sports. The ranking is performed by the total number of articles associated with a particular project among the projects that began in 2007 - only research articles published in journals indexed in Currents Contents were counted, up until March 1st, 2009 (web address: <http://bib.irb.hr/statistika?sto=p&period=2007&chset=ASCII&lang=EN>). The number of articles is the total number of scientific papers appearing in journals indexed in Currents Contents published on a particular project in 2008. 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.

	2005	2006	2007	2008	2008 / 2007 (%) increased	2008 / 2005 (%) increased
Revenue from the Ministry of Science Education and Sports (€)	17.293.472	20.072.940	23.090.639	25.818.444	11.8	49.29
Other revenue (international and industrial projects, services etc.) and donations (€)	1.890.592	2.311.744	3.671.788	3.486.303	-5.3	84.4
total	19.184.064	22.384.684	26.762.427	29.304.747	9.5	52.7
Employees						
Scientific staff	325	317	320	322	0.6	-0.9
post-doctoral students	30	40	42	53	26.2	76.7
Ph.D. students	159	158	177	155	-12.4	-2.5
Technicians and other	127	134	127	145	14.2	14.2
administration and maintenance	174	176	174	180	3.4	3.4
total	815	825	840	855	1.8	4.9

Table 1. Comparison of RBI Revenues (€) and employment during 2005-2008.

Field of Science - Number of National Projects in the Field	Project Title	Principal Investigator	Number of CC Articles Published in 2008
BIOLOGY - 77	Regulatory mechanisms of photosynthesis and plastid differentiation	Hrvoje Fulgosi	6
	Cell response to cytotoxic agents and resistance development	Maja Osmak	1
PHYSICS - 85	Physics and application of nanostructures and bulk matter	Krešimir Furić	17
	Fundamental interactions in elementary particle physics and cosmology	Branko Guberina	12
	Nuclear structure and reactions: experimental approach	Suzana Szilner	6
	Basic properties of nanostructures and defects in semiconductors and dielectrics	Branko Pivac	10
	Thin films of novel amorphous or nanostructured materials	Nikola Radić	5
	Ion beam interactions and nanostructures	Milko Jakšić	9
	Massive neutrinos and astroparticles: from particle physics to cosmology	Ante Ljubičić	5
GEOSCIENCES - 65	Interactions of trace metal species in an aquatic environment	Ivanka Pižeta	9
	Nature of organic matter, interaction with traces and surfaces in environment	Zlatica Kozarac	4
	Radionuclides and trace elements in environmental systems	Delko Barišić	3
CHEMISTRY - 73	Synthesis and microstructure of metal oxides and oxide glasses	Svetozar Musić	10
	Electroanalytical research on microcrystals and traces of dissolved substances	Milivoj Lovrić	12
	Self-Assembly in gels and synthesis of functional hybrid materials	Mladen Žinić	8

	NMR Spectroscopy and Modelling of Bioactive Molecules	Dejan Plavšić	5
	Broensted and Lewis acids and bases in chemistry and biochemistry	Zvonimir Maksić	2
	Molecular structure and dynamics in systems containing paramagnetic particles	Boris Rakvin	9
	Spectroscopy, chemical properties and reactions of biologically active molecules	Branka Kovač	9
TECHNICAL SCIENCE - 28	Multispectral data analysis	Ivica Kopriva	3
FUNDAMENTAL MEDICAL SCIENCES - 175	The role of different cell death responses to DNA-damage treatment	Marijeta Kralj	9
	Pharmacogenomics and proteomics of serotonergic and catecholaminergic system	Dorotea Mück-Šeler	7
	Molecular basis and treatment of psychiatric and stress related disorders	Nela Pivac	6
	Molecular characteristic of myofibroblasts derived from Dupuytren's contracture	Krešimir Pavelić	11
	Gene therapy of tumors by modulating the molecules of immune system	Jasminka Pavelić	5
	Lipids, free radicals and their messengers in integrative oncology	Neven Žarković	5
	Molecular genetics and pharmacogenetics of gastrointestinal tumors	Sanja Kapitanović	5
	Aberrant DNA methylation in HPV associated lesions	Magdalena Grce	4
	Serotonergic neurotransmission: genes, proteins and behavior	Branimir Jernej	3

Table 2. Publication results of RBI fundamental research projects ranked among the top 15% Croatian projects in their respective field.

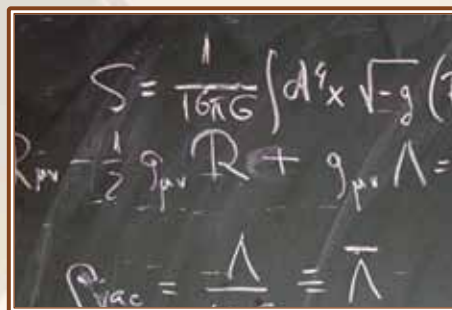


DIVISIONAL ORGANIZATION

Head: Branko Guberina

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

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



TOP ACHIEVEMENTS

Thermodynamics of Dark Energy

Thermodynamic properties of dark energy have been analyzed using the formalism of field theory at finite temperature. In particular, the formalism has been applied to a purely kinetic type of k-essence. It has been shown quite generally that the entropy associated with dark-energy is always greater than or equal to zero. Hence, contrary to often stated claims, a violation of the null energy condition (phantom dark energy) does not necessarily yield negative entropy (Bilić, 2008).

OVERVIEW OF THE DIVISION

The research performed in the Division is mainly concerned with the theoretical investigation of high-energy physics, such as particle physics, general and mathematical physics, astroparticle physics and cosmology. In addition, there is substantial research activity in condensed matter physics. A special activity in the Division is the nature of medical modelling in life science and the application of nonlinear statistical methods in biomedicine. In 2008, 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.

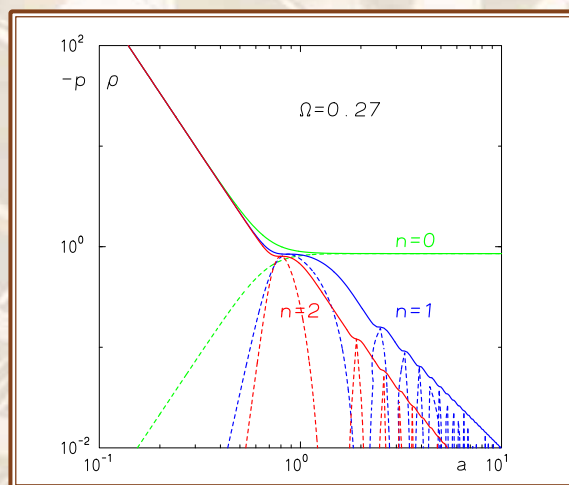


Figure 1. Evolution of the background density and pressure in the tachyon condensate cosmological model.

Improved QCD Light-cone Sum Rule

An improved QCD light-cone sum rule (LCSR) calculation of the $B \rightarrow K$ and $B_s \rightarrow K$ form factors by including SU(3)-symmetry breaking corrections is presented. By applying the method of the direct integration in the complex plane, the analytical extraction of the imaginary parts of LCSR hard-scattering amplitudes becomes unnecessary and therefore the complexity of the calculation is greatly reduced (Duplanić and Melić, 2008).

Noncommutative chiral models

In the noncommutative chiral gauge theories the 4-fermion vertices are shown to be finite. The 4psi vertices appear in linear order in quantization of the theta-expanded noncommutative gauge theories whereas in all previously considered models, based on Dirac fermions, the 4psi vertices were divergent and nonrenormalizable (Burić et al., 2008).

Deeply virtual Compton scattering

Combining dispersion and operator product expansion techniques, the conformal partial wave decomposition of the virtual Compton scattering amplitude has been derived in terms of complex conformal spin to twist-two accuracy. The perturbation theory predictions for the deeply virtual Compton scattering amplitude are presented in next-to-leading order for both the conformal and modified minimal subtraction schemes. Within a conformal subtraction scheme, where predictive power of conformal symmetry is exploited, the radiative corrections are presented up to next-to-next-to-leading order accuracy (Kumerički et al., 2008).

Noncommutative spaces

Kappa-Minkowski and generalized kappa-deformed spaces are investigated. We

developed a systematic study for constructing realizations of noncommutative spaces. Star product and Drinfeld twist operator are represented in terms of the coproduct (Meljanac, Samsarov et al., 2008; Meljanac and Krešić-Jurić, 2008). Twisted statistics of kappa-Minkowski space is analysed.

Integrable systems and applications in physics

A new analysis of the mechanism of electronic capture by polar molecules has been presented. This analysis is based on theory of self-adjoint extension and the results show that a polar molecule can form a bound state with electrons even when its dipole moment is less than the critical value of 1.63×10^{-18} esu cm (Giri et al., 2008). A rational Calogero model with additional interaction of Coulomb type has been studied, and it was shown that for certain values of the constants of interaction the system allows for one-parametric family of self-adjoint extensions which lead to novel solutions of this model (Basu-Mallick et al., 2008).

Homolumo gap and matrix model

We discuss a dynamical matrix model by which probability distribution is associated with Gaussian ensembles from random matrix theory, and interpret the matrix M as a Hamiltonian representing interaction of a bosonic system with a single fermion. We show that a system of second-quantized fermions influences the ground state of the whole system by producing a gap between the highest occupied eigenvalue and the lowest unoccupied eigenvalue (Andrić et al., 2008).

Enhanced van der Waals interaction at interfaces

The excitation of surface polaritons by a decaying atom or molecule and their subsequent conversion into the radiation (photons) is at the core of surface-enhanced op-

tical processes such as fluorescence and Raman scattering. We have considered the dispersion interaction between an excited and a ground-state atom near an interface under the condition of resonant coupling of the excited atom to surface polaritons. We have demonstrated that the nonretarded atom*-atom interaction energy at a vacuum-medium interface can be enhanced by several orders of magnitude in comparison with the van der Waals interaction energy of the two isolated atoms. This promotes the van der Waals interaction as another example of the surface enhanced phenomena (Tomaš, 2008).

From degree correlations to feedback in directed complex networks

The reciprocity is a natural measure of feedback in complex systems representable as directed complex networks. The role of one-vertex and two-vertex degree correlations in explaining the value of reciprocity has been studied analytically and in computer simulations using newly developed randomization algorithms. The hierarchy of importance of various degree correlations for the understanding of reciprocity has been established and verified on a number of important empirical complex networks comprising world trade webs, neural networks of *Caenorhabditis elegans*, cortical networks, food webs and Wikipedia networks (Zamora-López et al., 2008).

EDUCATION

In 2008, the members of the Division continued to be involved in lecturing undergraduate and graduate courses at the University of Zagreb, mostly at the Faculty of Science. A number of students completed their B. Sc., M. Sc. and Ph. D. theses.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Sciences, Education and Sports

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

Programs supported by the Ministry of Sciences, Education and Sports

1. High energy physics, gravity and cosmology, Branko Guberina.

Research, developmental and international projects

1. QCD sum rules for exclusive decays of heavy hadrons, Blaženka Melić (International Research Project promoted by the Alexander von Humboldt Foundation, with principal investigators from RBI and University of Siegen, Germany)
2. Aspects of Calogero models, noncommutative geometry and quantum physics, Stjepan Meljanac (Indo-Croatian Programme of Cooperation in Science and Technology for collaboration between RBI-ZTF, Saha Institute of Nuclear Physics, Calcutta, and Institute of Mathematical Sciences, Chennai, India)
3. Nonabelian Cohomology and Applications in Geometry, Algebra and Physics, Zoran Škoda (International collaboration between RBI-ZTF

and Universität Hamburg, LMU München and Universität Göttingen, Germany)

4. Tools and Precision Calculations for Physics Discoveries at Colliders, Josip Trampetić (collaboration to the FW 6 EU RTN Network HEPTOOLS, no. MRTN-CT-2006-035505)

SELECTED INVITED LECTURES

1. Andraši A. Divergences in Coulomb gauge QCD, A Triangle Workshop in Theoretical Physics, Heviz, Hungary, January 23-25, 2008.
2. Škoda Z. Categorified actions and 2-representations, Functional analysis X Conference, Dubrovnik, June 29 - July 5, 2008.
3. Melić B. $B \rightarrow \pi$ and $B(s) \rightarrow K$ form factors and Vub determination, 34th International Conference on the High Energy Physics ICHEP2008, Philadelphia, USA, July 29 – October 5, 2008.
4. Jonke L. $U(1)$ gauge field theory on kappa-Minkowski space, Supersymmetry and non-commutative quantum field theory, Workshop in Memoriam Julius Wess, Vienna, Austria, December 4-6, 2008.

SELECTED ORGANIZED CONFERENCES

1. Workshop on Black Holes in General Relativity and String Theory, V. Lošinj, Croatia, August 24-30, 2008, Larisa Jonke and Neven Bilić, members of the Organizing Committee
2. 3rd Croatian-Hungarian-Austrian Meeting – Non Abelian Theories, Hot Matter and Cosmology, Rab, Croatia, August 30 – September 4, 2008, organized by Ivan Dadić

SELECTED PUBLICATIONS

1. Andrić I, Jonke L, Jurman D, Nielsen H B. Homolumo gap and matrix model. Phys Rev D 2008: 77: 127701.
2. Basu-Mallick B, Gupta K S, Meljanac S, Samsarov A. Inequivalent quantization of the rational Calogero model with a Coulomb type interaction. Eur Phys J C 2008: 58: 159.
3. Bilić N. Thermodynamics of k-essence, Phys Rev D 2008: 78: 105012.
4. Burić M, Latas D, Radovanović V, Trampetić J. Absence of the 4psi divergence in non-commutative chiral models, Phys Rev D 2008: 77: 045031.
5. Duplančić G, Melić B. $B(s) \rightarrow K$ form factors: an update of light-cone sum rule results. Phys Rev D 2008: 78: 054015.
6. Giri P R, Gupta K S, Meljanac S, Samsarov A. Electron capture and scaling anomaly in polar molecules. Phys Lett A 2008: 372: 2967.
7. Kumerički K, Müller D, Passek-Kumerički K. Towards a fitting procedure for deeply virtual Compton scattering at next-to-leading order and beyond. Nuclear Phys B 2008: 794: 244.
8. Meljanac S, Krešić-Jurić S. Generalized kappa-deformed spaces, star products and their realizations. J Phys A 2008: 41: 235203.
9. Meljanac S, Samsarov A, Stojić M, Gupta K S. Kappa-Minkowski spacetime and the star product realizations. Eur Phys J C 2008: 53: 295.
10. Tomaš M S. Enhanced van der Waals interaction at interfaces. J Phys A Math Theor 2008: 41: 164020.
11. Zamora-López G, Zlatić V, Zhou C, Štefančić H, Kurths J. Reciprocity of networks with degree correlations and arbitrary degree sequences. Phys Rev E 2008: 77: 016106.

Division of Experimental Physics

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

DIVISIONAL ORGANIZATION

Head: Alfred Švarc (until Sept 27, 2008);
Tome Antičić (from Nov 20, 2008)

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

- ⇒ Laboratory for nuclear reactions, Neven Soić
- ⇒ 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
- ⇒ Laboratory for hadron physics in between experiments and QCD models, Alfred Švarc



are over 60 staff members, including more than 30 Ph.D. students. They are involved in numerous experiments and experimental complexes abroad and in Croatia, and maintain a strong performance in both basic and applied physics research. The Division, due to its excellent international reputation, received a large fraction of its financing from sources other than Ministry of Sciences Education and Sports which was used, among others, to significantly enhance its experimental capabilities.

TOP ACHIEVEMENTS

Ion beam assisted formation and modification of nanodiamonds

Implantation of 1-2 MeV carbon ions was successfully applied in process of carbon nanocrystal formation in amorphous silica, while changes in luminescence properties of nanodiamonds embedded in PDMS was studied using irradiation by 2 a MeV proton beam (Borjanović et al., 2008).

A technique for patterning radiation damage using heavy ion microbeam developed previously on silicon pin diodes (Figure 1) has now been applied to modify the electronic properties of diamond for the first time.

OVERVIEW OF THE DIVISION

The Division of Experimental Physics is focused on experimental and theoretical nuclear and particle physics, astrophysics, and recently also in quantum information. There

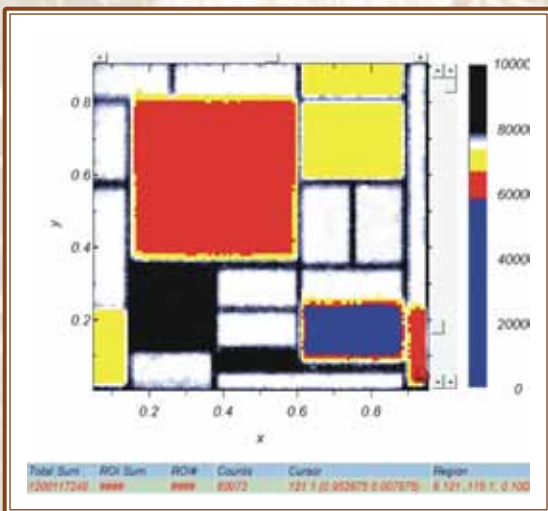


Figure 1. Radiation damage structures induced in Si pin diode by 7 MeV carbon ions in a form of Piet Mondrian painting. Diode was imaged by IBIC technique using the same ions. Charge collection efficiency decreases from the highest (black) to the lowest (blue).

pp→WZ analysis for the CMS Collaboration at LHC

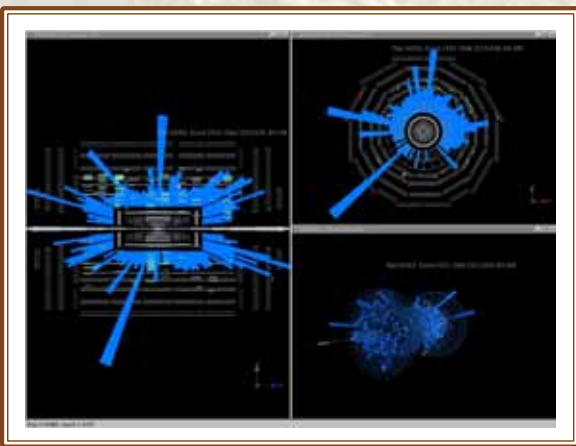


Figure 2. One of the first images from CMS, showing the debris of particles picked up in the detector's calorimeters and muon chambers.

The CMS potential for the observation of the pp→WZ reaction was investigated using simulated signal and background samples. New data-driven methods for the background determination have been developed. A member of our group has been selected as convenor for all multiboson analyses in the CMS Collaboration. We have also participated in the analysis of the first cosmic muons measured by CMS.

Energy scans at the NA49 SPS experiment

An energy scan in Pb+Pb collisions at the NA49 detector at the CERN-SPS was performed to understand the crossover region of the transition from normal matter to the quark-gluon plasma phase. Statistical hadron gas models provided a reasonable description of the Λ and Ξ yields, while string hadronic models failed to match the Ξ multiplicities. Phi meson energy dependence was shown to be compatible with the assumption that partonic degrees of freedom set in at low SPS energies. At 30A GeV a change of the energy dependence for yields as well as for the shape of the transverse mass spectra is observed, compatible with the prediction that the threshold for production of a state of deconfined matter at the early stage of the collisions is located at low SPS energies (Alt et al., 2008).

Natural isotopes in environmental studies and radiocarbon dating

The new system for graphite preparation of micro-sized samples for ^{14}C measurement by AMS technique was validated at the SUERC, Scotland. Dating of prehistoric and medieval sites from Croatia and Slovenia by the LSC method continued. Carbon exchange processes in atmosphere, water and lake sediments was studied together with measurements of stable isotopes to assess possible anthropogenic contamination in Karst systems. The monitoring of ^3H activity in precipitation in Croatia and Slovenia continued, as did that of biological samples and atmospheric CO_2 near the nuclear power plant Krško. A training course dedicated to dating methods within the regional IAEA technical project RER/1/006 was organized in Zagreb. A workshop dedicated to valorization of monumental heritage and characterization of constructive materials was organized in Split.

Scattering of protons and deuterons at 135 MeV revisited

Study of proton and deuteron scattering allows the inferring of information on the three-nucleon force for the smallest nuclear system possible. There has been a strong discrepancy among existing data at 135 MeV/nucleon (Figure 3). A precise measurement at this energy for the $^2\text{H}(p,d)p$ and $^1\text{H}(d,d)p$ reactions have been carried out using polarized beams and liquid targets. The data differ significantly from previous measurements and consistently follow the energy dependence as expected from an interpolation of published data (Gašparić et al., 2008).

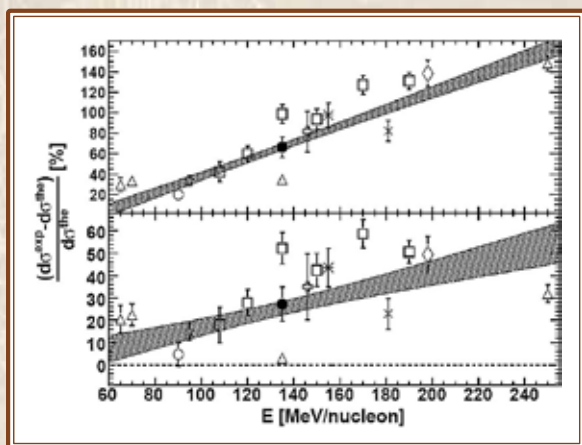


Figure 3. Difference between theory and the measured cross sections for the elastic $p+d$ reaction. The top graph shows the results from a standard calculation, while the bottom includes an additional Δ isobar. Solid circles are this work. Although the discrepancy is reduced in the lower panel, inconsistencies remain.

Exotic nuclear phenomena

The largest amount of knowledge in nuclear physics is about nuclei close to the valley of stability, but recent studies have moved towards the driplines and more exotic nuclear phenomena. Our current studies concern proton-rich light nuclei and many-centre cluster structures in the neutron-rich light nuclei. Design and construction of the detector array for nuclear structure and reaction research has been extended by inclusion of new electronic devices (FP7 project

CLUNA). With aim to study the properties of the nuclear systems at extreme conditions, the measurements at the INFN-LLN Legnaro, INFN-LNS Catania and UCL Louvain-la-Neuve have been performed and new experiments proposed by our group have been approved at the INFN-LLN and GANIL Caen facilities.

Search for solar hadronic axions

Axions (pseudoscalars that arise in models resolving the strong CP problem by the Peccei-Quin mechanism) could also explain the mystery of dark matter in the Universe. We developed a new approach to search for hadronic axions that is free from the large uncertainties associated with the estimation of the flavor-singlet axial-vector matrix element.

Large extra dimensions

In an experiment performed at the RBI we did not observe the bulk vector boson signal from the Sun. This result rules out the possibility of observing any signal at the LHC for two additional space dimensions (Horvat et al., 2008).

Holographic dark energy

An extremely small entropy pertaining to holographic dark energy models is explained for the first time with the aid of the entanglement entropy for the subsystems (the cosmic horizon and the interior) to show that via quantum correlations this entropy may be responsible for the almost purity of the entire system (Horvat, 2008).

The holographic dark energy models, successful in describing the late-time dark energy universe, are shown to have conceptual problems when describing the earlier cosmological epochs, so that a reassessment of the whole concept is needed (Horvat, 2008).

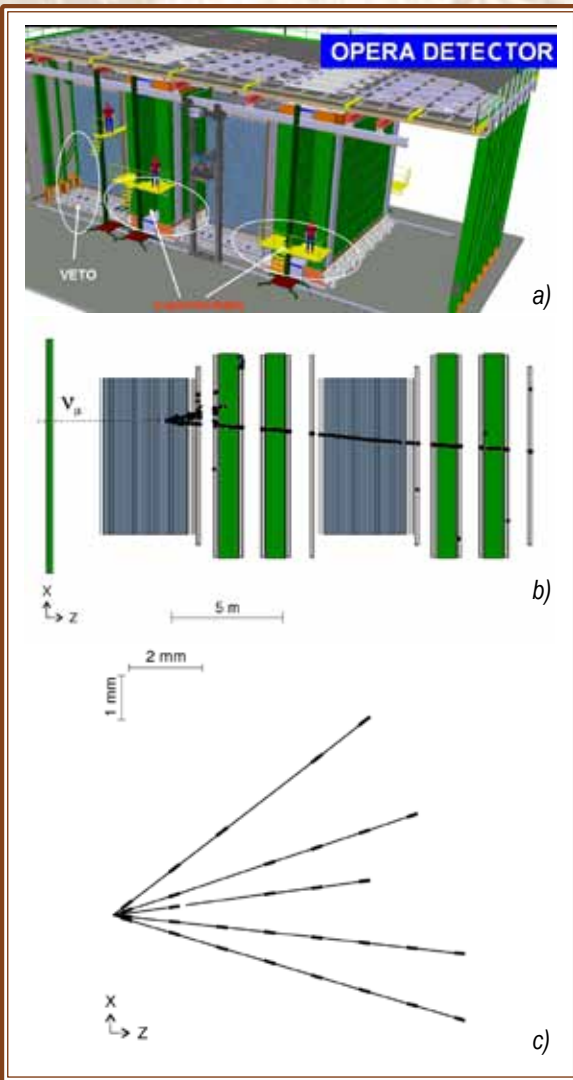


Figure 4. OPERA: (a) the detector, (b) a neutrino CC event (c) vertex tracks recorded.

OPERA neutrino oscillations experiment

Our scientists took part in data taking at OPERA (long-baseline experiment designed to investigate neutrino oscillations), which resulted in the first 1000 recorded neutrino events. They are also strongly involved in the electronics detector group and in data analysis.

Environmental Security of the Coastal Sea Floor

The detection and identification of improperly disposed ammunition, explosives and chemical weapons at the sea floor and pollution of coastal sea sediments are problems of growing concern. While polluted sediments present a threat to the marine ecosystem and to the public health, ammunition and CW agent dumps are a serious threat as well as possible objects of misuse. The research in this field has been established in LNAM (Valković et al., 2008). In 2007 we made the first prototype of the underwater system "Surveyor" containing a neutron generator, shielding and a gamma ray detector. In 2008 the "proof of principle" for the detection of explosive and chemical warfare agents has been established (Sudac et al., 2008).



Figure 5. Reported locations of ammunition on the floor of the Mediterranean (UNEP, 2007).

Matrix characterization in threat material detection processes

Matrix characterization is a key for the neutron prototype systems used for threat material inspection in cargo containers, landmine detection or underwater threat materials inspections. For this purpose, the chemical composition of samples of container cargo, soil and sea sediment have been analyzed using the Fast Neutron Activation Method with Associate Alpha Particle and Energy Dispersive X-Ray Fluorescence (Obhodaš et al., 2008).



Figure 6. The prototype of the underwater system "Surveyor" containing neutron generator.

Poles as a true resonance signal

The present manner in which the Particle Data Group is parameterizing nucleon resonances in terms of Breit-Wigner parameters have been criticised as being inherently model dependent. An appeal to change the harmful practice and use scattering matrix pole parameters instead is issued, and two new, model independent ways to extract pole parameters from partial wave data are presented.

The Crystal Ball Spectrometer

A new experimental program at the Mainz Microtron (MAMI) facility consists of the Crystal Ball, the TAPS detector and a central tracker. The Crystal Ball collaboration is

devoted to experiments using energy tagged Bremsstrahlung photons and its major experiments are the measurements of the anomalous magnetic moment of the Delta resonance, of the mass of the eta-meson and double pion production at threshold, and others (Tarbet et al., 2008).

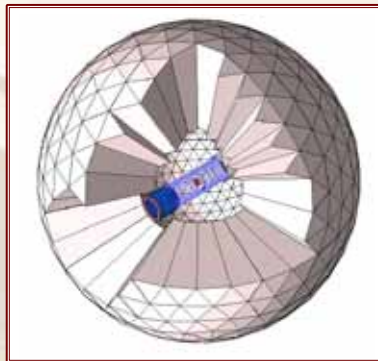


Figure 7. The Crystal Ball Spectrometer.

NEW EQUIPMENT

With the support of the EU FP6 project RBI-AF two quadrupole magnets were added to the existing ion microprobe focussing facility to enable focussing of heavy ion beams, enabling focusing to submicron spot sizes of ions of up to 15 MeV mE/q² rigidity.

A laboratory for research in quantum information has been formed for the first time in Croatia. A setup for study of polarization entangled photon pairs was built and used to measure quantum efficiency and single photon timing resolution of a photon detector (constructed in the laboratory).

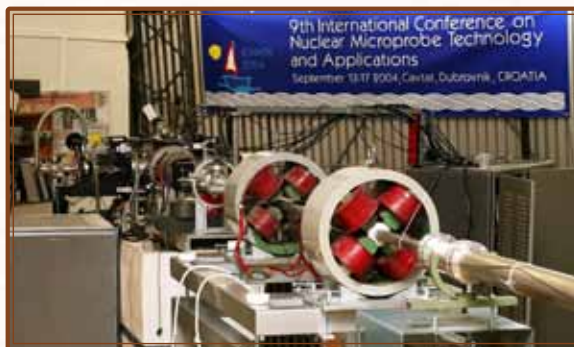


Figure 8. Series of five quadrupole magnets installed at the microprobe beam line to form spaced quintuplet system for ion beam focusing.

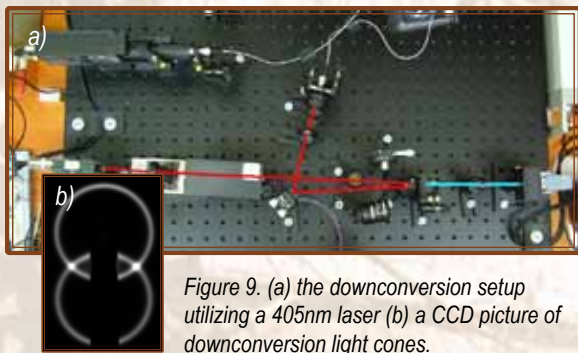


Figure 9. (a) the downconversion setup utilizing a 405nm laser (b) a CCD picture of downconversion light cones.

EDUCATION

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

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sports

1. Experimental research of the nucleus: nuclear structures and reactions, Suzana Szilner
2. Ion beam interactions and nanostructures, Milko Jakšić
3. Hadronic physics and QCD, Ivan Supek
4. Heavy-ion physics, Zoran Basrak
5. Massive neutrinos and astro-particles: from particle physics to cosmology, Ante Ljubičić
6. Experimental physics at LHC energies, Krešo Kadija
7. Experiments in quantum communication and quantum information, Mario Stipčević
8. Photon-atom interactions and correlations, Tihomir Surić
9. Natural isotopes of weak activities and development of instrumentation, Bogomil Obelić
10. Development and application of nuclear analytical methods, Jasmina Obhodaš
11. Development of methods for control of illicit threat material trafficking, Dario Matika and Davorin Sudac
12. Nuclear interactions, Ivo Šlaus
13. Development and application of nuclear methods for investigation and protection of cultural heritage, Vladan Desnica

Programs supported by the Ministry of Science, Education and Sports

1. High energy experimental physics within and beyond the standard model, Krešo Kadija
2. Water in Karst - dynamics, geochemistry and isotopic processes, Bogomil Obelić

Research, developmental and international projects

1. CLUustering phenomeNA in nuclear physics: strengthening of the Zagreb - Catania - Birmingham partnership (CLUNA), Neven Soić (FP7-REGPOT-2007-3 International Cooperation - Coordination and Support action, project number 203200)
2. Preparation of carbon samples for ^{14}C dating by the AMS technique - AMS-14C, Ines Krajcar Bronić (EC FP6 program INCO-CT-2006-043584)
3. Upgrade of the RBI Tandem Accelerator Facility – RBI-AF, Stjepko Fazinić (EC FP6 program INCO Contract 043630)
4. EUROpean Nuclear Structure Integrated Infrastructure Initiative – EURONS, Zoran Basrak (EC FP6 program, Contract 506065)
5. Development of frozen spin polarized target for Crystal Ball Collaboration at MAMI, Ivan Supek (University of Mainz for EU program I3HP TNA Contract)
6. TRAINMONHER - Valorization of Monumental Heritage through Higher Education and Professional Training. Socioeconomic study and analysis of National Policies on EU-MED-DEV countries and EC Directives, Bogomil Obelić (EU FP6 project INCO-CT-2006-518697)
7. Eritr@C, European Riposte against illicit trafficking, Davorin Sudac (EU programme "Prevention of and fight against crime", Agreement no. JLS/2007/ISEC/550)
8. EURITRACK, European Illicit Trafficking Countermeasures Kit, Vladivoj Valković, (EU FP6- Specific Targeted Research or Innovation Project)
9. Nuclear Techniques for the Protection of Cultural Heritage Artifacts in the Mediterranean Region, Stjepko Fazinić (National Coordinator, IAEA regional project RER/1/006)
10. Measurements of differential cross sections for elastic scattering of ^1H and ^4He ions from selected light elements, Ivančica Bogdanović Radović (IAEA Research Contract 13269/RO)

11. Heavy ion acceleration in 1.0 and 6.0 MV electrostatic accelerators, Milko Jakšić (IAEA Research Contract 13127/RO)
12. Upgrade of PIXE and STIM imaging capabilities at Zagreb nuclear microprobe, Mladen Bogovac (IAEA Research Contract 13258/RO)
13. Characterization of inorganic pigments used by selected painter(s) by nuclear microprobe, Stjepko Fazinić (IAEA Research Contract 13050/RO)
14. Modification of electronic properties in insulators using nuclear microprobe, Marko Karlušić (IAEA Research Contract 12925/RO)
15. Improvements of ERDA technique using TOF spectrometer, Zdravko Siketić (IAEA Research Contract 14580)
16. Application of isotope techniques in investigation of water resources and water protection in the Karst area of Croatia, Nada Horvatinčić, (In co-operation with the University of Rijeka; IAEA Technical co-operation project CRO/8/006)
17. Using Isotope Tracers as a Tool for Groundwater Vulnerability Assessment in the County of Split, Dalmatia, Nada Horvatinčić (In co-operation with the University of Rijeka; IAEA Technical co-operation project CRO/8/007)
18. Isotope methods for management of drinking water resources, Nada Horvatinčić (IAEA regional project RER/8/012)
19. Photon detector for applications in quantum experiments, diagnostic and analytical methods, Mario Stipčević (Technological project financed by Croatian Institute of Technology)
20. Study of advantages and limitations of Si pin diodes as radiation detectors by ion beam methods, Milko Jakšić (bilateral project with Hungary)
21. Heavy ion physics, Roman Čaplar (International collaboration project RBI-KFKI Research Institute for Particle and Nuclear Physics, Budapest via Croatian (HAZU) and Hungarian Academy of Science)
22. Heavy-ion reaction dynamics studies, Zoran Basrak (bilateral research project Croatia-India)
23. Experiments in quantum communication and quantum information, Mario Stipčević (A bilateral research project Croatia-Germany (DAAD), Contract number: 098-0352851-2873)
24. OPERA collaboration, Ante Ljubičić (International collaboration between RBI, CERN (Switzerland) and LNGS (Gran Sasso, Italy))
25. Axion Solar Telescope (CAST) experiment, Milica Krčmar (International collaboration between RBI and CERN, Switzerland)

26. Precise Measurement of the $\Pi^+ \rightarrow e^+ \nu$ Branching Ratio, Ivan Supek (International Collaboration between RBI and University of Virginia, Charlottesville, USA)

SELECTED INVITED LECTURES

1. Basrak Z. Selected effects of the NN cross section on heavy-ion dynamics, Workshop on Nuclear Symmetry Energy at Medium Energies, Catania and Militello in Val di Catania, Italy, May 29-31, 2008.
2. Bogdanović Radović I. 3D imaging of light elements using elastic scattering coincidence technique, 11th International Conference on Nuclear Microprobe Technology and Applications Debrecen, Hungary, July 20-25, 2008.
3. Brigljević V. Measurement of diboson production in early LHC data, Physics at LHC 2008, Split, Croatia, September 29-October 4, 2008.
4. Jakšić, M. Accelerators of the Ruđer Bošković Institute: From the successful history to promising future, CoNuSS-2008, Belgrade, Serbia, September 22-25, 2008.
5. Kiš M. New FOPI MMRPC ToF Barrel, Deutsche Physikalische Gesellschaft Frühjahrstagung, Darmstadt, March 10-14, 2008.
6. Lakić B (for the CAST collaboration). Search for solar axions with the CAST experiment. Identification of Dark Matter 2008, Stockholm, Sweden, August 18-22, 2008.
7. Obelić B. Dating Techniques in Monumental Heritage, Training course on Monumental Heritage within the EU project INCOCT-2006-518697 "TRAINMONHER", Marrakech, Morocco, April, 14-18, 2008.
8. Obelić B. Técnicas de datación en el patrimonio monumental, Universidad Michoacana de San Nicolás de Hidalgo, Morelia (México), June 11, 2008.
9. Obhodaš J, Sudac D, Valković V. Matrix characterization in threat material detection processes. 20th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas, August 10-15, 2008.
10. Szilner S. Nucleon-nucleon correlation effects in multinucleon transfer reactions, GAMMAPOOL Workshop, Paris, May 27-30, 2008.
11. Szilner S. Quasi-elastic reactions : a survey on recent results with PRISMA-CLARA, Fusion08 - New Aspects of Heavy Ion Collisions Near the Coulomb Barrier, Chicago, Illinois, USA, September 22-26, 2008.

12. Valković V, Obhodaš J, Sudac D, Matika D. Environmental Security of the Coastal Sea Sediments, 20th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas, August 10-15, 2008.
13. Siketić. Quantitative analysis of hydrogen using TOF ERDA spectroscopy, 20th International Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas, August 10-15, 2008.
14. Bogdanović-Radović I. Materials analysis and modification using MeV heavy ions NIS Colloquium, Materials analysis and Modification by Ion Beams, University of Torino, Italy, December 22, 2008.

SELECTED ORGANIZED CONFERENCES

The thirteenth biennial European X-ray Spectrometry Conference was held from 16th to 20th June 2008 in Cavtat (EXRS-2008). Organized by RBI and co-chaired by M. Jakšić and S. Fazinić, the conference was attended by 280 scientists from 41 countries and 22 industrial exhibitors. On the basis of regular review procedure, selected papers were published in the X-Ray Spectrometry journal.

The Crystal Ball Workshop was organized by I. Supek, and held in Dubrovnik from April 6 to 9, 2008 with attendance of over 50 scientists from all over the world. It was devoted to the development of experiments to investigate the strong interaction, rare decays and symmetry breaking, as well as to provide new insights in physics beyond the Standard Model.

SELECTED PUBLICATIONS

1. Borjanović V, Lawrence WG, Hens S, Jakšić M, Zamboni I, Edson C, Vlasov I, Shenderova O, McGuire GE. Effect of proton irradiation on photoluminescent properties of PDMS-nanodiamond composites. *Nanotechnology* 2008: 19: 455701-1.
2. Bogdanović Radović I, Siketić Z, Jakšić M, Gurbich A. Measurement and parametrization of proton elastic scattering cross-sections for nitrogen. *Journal of Applied Physics* 2008: 104: 074905-1.
3. Horvat R, Kekez D, Krečak Z, Ljubičić A. Constraining theories of low-scale quantum gravity by nonobservation of the bulk vector boson signal from the Sun. *Phys Rev D* 2008: 78: 127101.
4. Wu Q et al., (RBI-NOMAD collaboration: Lakić B, Ljubičić A, Stipčević M). A precise measurement of the muon neutrino-nucleon inclusive charged current cross section off an isoscalar target in the energy range $2.5 < E_\nu < 40$ GeV by NOMAD. *Phys Lett B* 2008: 660: 19.
5. Horvatinčić N, Barešić N, Babinka S, Obelić B, Krajcar Bronić I, Vreča P, Suckow A. Towards a deeper understanding how carbonate isotopes (^{14}C , ^{13}C , ^{18}O) reflect environmental changes: A study with recent ^{210}Pb -dated sediments of the Plitvice Lakes, Croatia, *Radiocarbon* 2008: 50: 233.1.
6. Horvat R. On the internal consistency of holographic dark energy models. *JCAP* 2008: 10: 022.
7. Prakhov S, et al., (Supek I). Measurement of the invariant-mass spectrum for the two photons from the $\eta \rightarrow \pi^0 \gamma \gamma$ decay. *Phys Rev C* 2008: 78: 015206.
8. Curtis N, et al., (Soić N). Breakup reaction study of the Brunnian nucleus ^{10}C , *Phys Rev C* 2008: 77: 021301-5.
9. Valiente-Dobón JJ et al. (Szilner S.), Spectroscopy of neutron-rich $^{59-63}\text{Mn}$ isotopes. *Phys Rev C* 2008: 78: 024302-1.
10. Ramazani-Moghaddam-Arani A, et al. (BINA Collaboration-IRB: Gašparić I). Elastic proton-deuteron scattering at intermediate energies. *Phys Rev C* 2008 : 78: 014006.
11. Ceci S, Stahov J, Švarc A, Watson S, Zauner B. Resolution of the multichannel anomaly in the extraction of S-matrix resonance-pole parameters. *Phys Rev D* 2008: 77: 116007-1.
12. Ceci S, Švarc A, Zauner B, Manley M, Capstick S. Model-independent resonance parameter extraction from the trace of K and T matrices. *Phys Lett B* 2008: 659: 228.
13. Alt C et al. (NA49 Collaboration-IRB: Antičić T, Kadija K, Nikolić V, Šuša T. Energy dependence of Lambda and Xi production in central Pb+Pb collisions at 20A, 30A, 40A, 80A, and 158A GeV measured at the CERN Super Proton Synchrotron. *Phys Rev C* 2008: 78: 034918-1.

Chapters in books

1. Lakić B, Horvat R, Krčmar M. Axions and Large Extra Dimensions. In: *Axions: Theory, Cosmology, and Experimental Searches. Lecture Notes in Physics 741*. Editor: Kuster M et al. Springer, Berlin Heidelberg, 2008, pp 73-82.

Division of Materials Physics

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

DIVISIONAL ORGANIZATION

Head: Nikola Radić

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

- ⇒ Laboratory for Semiconductors, Branko Pivac
- ⇒ Laboratory for Thin Films, Nikola Radić
- ⇒ Laboratory for Molecular Physics, Krešimir Furić



OVERVIEW OF THE DIVISION

The Division of Materials Physics is focused on fundamental and applied studies of physical parameters and processes that describe and connect the microscopic, mesoscopic and macroscopic properties of condensed matter and molecules. Nanoscience and nanotechnology has been the most active direction of both fundamental scientific research and developments in technology. Various kinds of nanophased materials have been produced by non-equilibrium thermodynamic processing (magnetron sputtering, ion implantation) and subsequent treatments (thermal annealing, ion bombardment), and characterized by different methods, including XRD, SAXS, Raman spectroscopy, electron microscopy, AFM etc. Fundamental research in the field of molecular and solid state physics placed special emphasis on vibrational spectroscopy of the wide range of

systems - from metals, semiconductors, and ceramics on one side, to molecular crystals and biological samples on the other. Finally, the strong nonlinear effects in laser-matter interaction, and the spontaneous and induced self-organization in condensed systems continue to be subjects of intensive research. During 2008 the results of research carried out in the Division were published in 28 contributions to the journals listed in Current Contents, with an average impact factor per paper of 1.85.

TOP ACHIEVEMENTS

Selected results in study of diamond nanocrystal formation in amorphous silica

Carbon ion implantation in amorphous silica, followed by annealing in a hydrogen-rich environment, leads to preferential formation of carbon nanocrystals with cubic diamond (c-diamond), face-centred cubic (*n*-

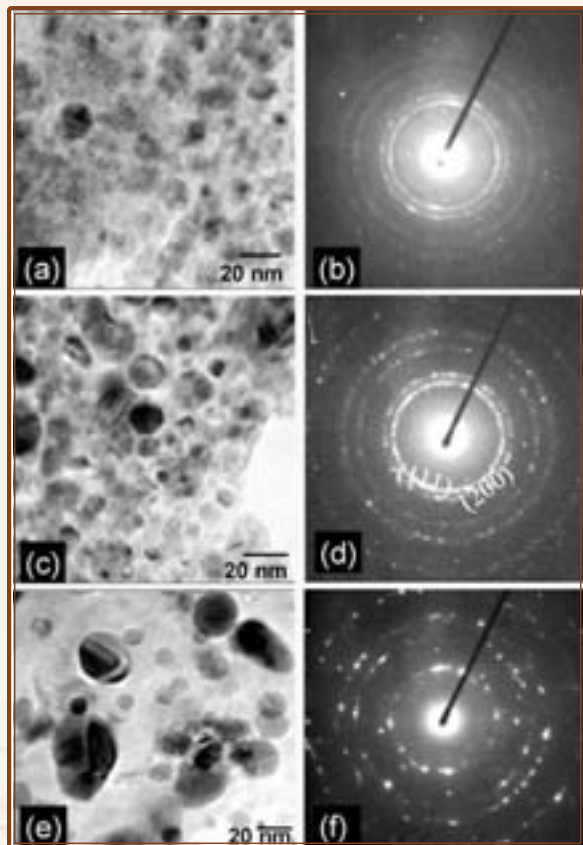


Figure 1. Transmission electron microscopy images (left side) and the corresponding selected area electron diffraction patterns (right side) of formed carbon nanocrystals after annealing. Observed phases depended on the implanted dose: [(a) and (b)] *i*-carbon nanophase was formed for $D3=1 \times 10^{17} \text{ C/cm}^2$; [(c) and (d)] *n*-diamond was formed for $D2=5 \times 10^{16} \text{ C/cm}^2$; and [(e) and (f)] cubic diamond was dominant and *n*-diamond was a minor phase for $D1=1 \times 10^{16} \text{ C/cm}^2$.

diamond), or simple cubic (*i*-carbon) carbon crystal lattices. The preferential formation of different carbon phases (diamond, *n*-diamond, or *i*-carbon) depends on implantation energy, implantation dose, and annealing conditions. Diamond nanocrystals formed at a relatively low carbon volume density are achieved by deeper implantation and/or lower implanted dose. Higher volume densities led to *n*-diamond and finally to *i*-carbon crystal formation. The optical properties of different carbon nanocrystal phases were significantly different (Buljan et al., 2008).

Raman scattering on quadrupolar vibrational modes of spherical nanoparticles

In contrast to the symmetrical mode, the coupling coefficients $C(\nu)$ of the quadrupolar vibrational modes of spherical nanoparticles embedded in a matrix consist of the longitudinal and transversal sound velocity contributions. Depending on the ratio of longitudinal and transverse sound velocities, these two contributions can interfere constructively or destructively resulting in enhancing or vanishing of some radial modes. The inverse problem of the determination of sound velocities of nanoparticles from the polarized low frequency Raman spectra by using the calculated $C(\nu)$ and known size distribution of the nanoparticles was demonstrated (Ristić et al., 2008).

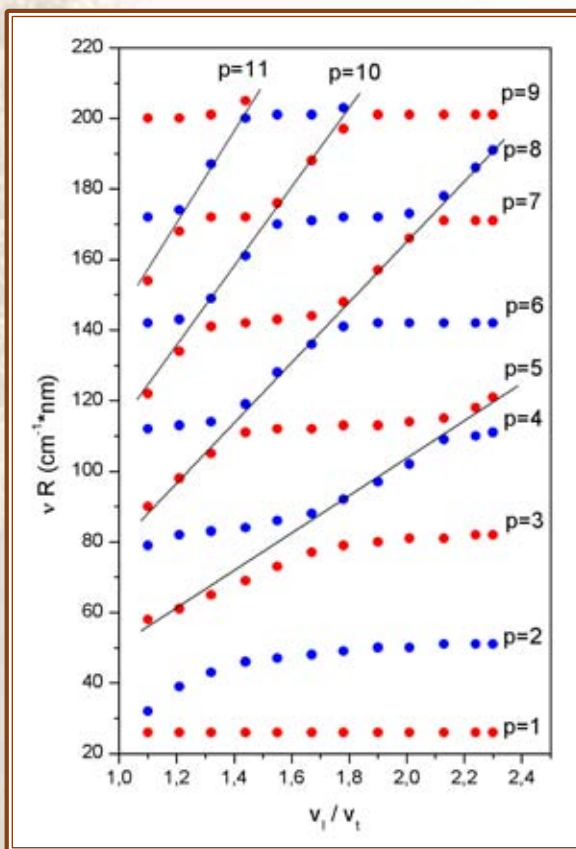


Figure 2. Calculated frequencies of the vibrational modes of a quasi-free spherical nanoparticle in dependence on the v_l/v_t ratio. The full lines mark the longitudinal spheroidal modes.

Low temperature resistivity of heavily boron doped LPVCD polysilicon thin films

Heavily boron δ -doped polysilicon samples were prepared by horizontal low-pressure chemical vapour deposition (LPCVD) at 750 °C for 1 h and were annealed at 1200 °C for 1 h. The resistivity was measured from room temperatures down to 2K. A $T^{1/2}$ dependence of the conductivity in an unusually wide temperature interval, even up to 80K was observed. Above 140K, the resistivity can be described by the $T^{3/2}$ dependence. The experimental results were analysed within the theories for the disordered metals (Žonja et al., 2008).

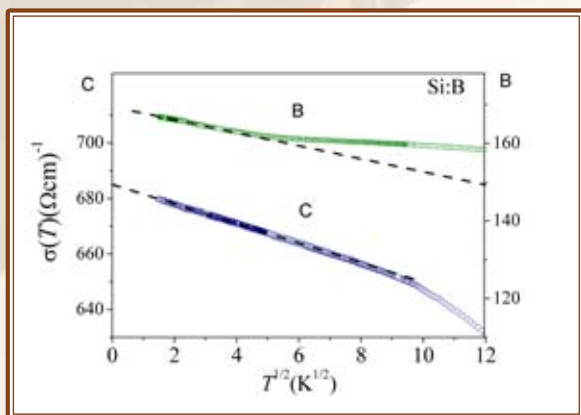


Figure 3. Conductivities of samples with different boron doping concentration (B and C) as a function of $T^{1/2}$. The samples beyond the critical concentration show metallic like behaviour. A rather wide interval of the $T^{1/2}$ dependence of the conductivity is attributed to the strong hole-hole interaction due to the high boron concentration. At higher temperatures, from 140 K for sample C, the resistivity can be described by the $T^{3/2}$ dependence, like in some amorphous materials.

Mount-Etna-Lava-Supported Nanocarbons for Oxidative Dehydrogenation Reactions

It was shown that the catalysis reaction rate in the oxidative dehydrogenation (ODH) for the production of butadiene from 1-butene, and styrene from ethylbenzene is much faster when the carbon nanofibers (CNF) supported on lava are used as catalyst in comparison

to the use of loose CNFs. Furthermore, the Raman spectrum after immobilization of the CNFs on the lava support shows only the bands characteristic to carbon and CNTs, and those bands remain after the ODH reaction (Figure 4a). A slight shoulder (D' band), typical for disordered carbon, which appeared after reactions is in agreement with the findings from high-resolution TEM (Figure 4b), where a slightly disordered surface structure on the CNFs was observed. Thus, a promising use of a huge, inexpensive natural resource in nanomaterials synthesis and in catalysis for production of butadiene and styrene is demonstrated (Su et al., 2008).

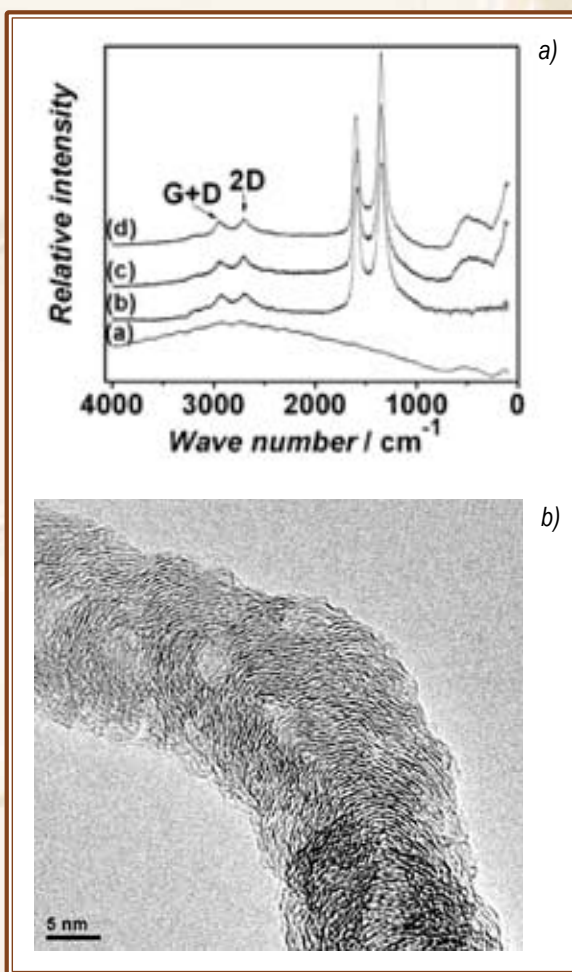


Figure 4. a) Raman spectra of (a) lava, (b) lava-CNFs before reaction, (c) lava-CNTs after ODH of ethylbenzene to styrene, and (d) lava-CNTs after ODH of butene to butadiene reaction. b) HRTEM images of CNFs on lava stone after ODH of ethylbenzene to styrene reaction.

Laser-induced convection nanostructures on SiON/Si interface

The homogenized beam of an excimer KrF laser has been used to form rectangular millimeter-scale holes of vertical walls in the $\sim 1 \mu\text{m}$ thick silicon-oxynitride (SiON) thin film deposited on a Si <111> wafer. At the same time, horizontal thermal gradient causes the formation of the nanoscale Marangoni convection structures at the SiON/Si interface. The inhomogeneous pattern of the roll structures can be divided into domains of regular, irregular and chaotic organization. Numerical simulation of the Marangoni domain roll structures based on the simple Swift-Hohenberg equation has reproduced all observed types of the roll organization, including those which show the evolution of dislocations from the Eckhaus instability (Maksimović et al., 2008).

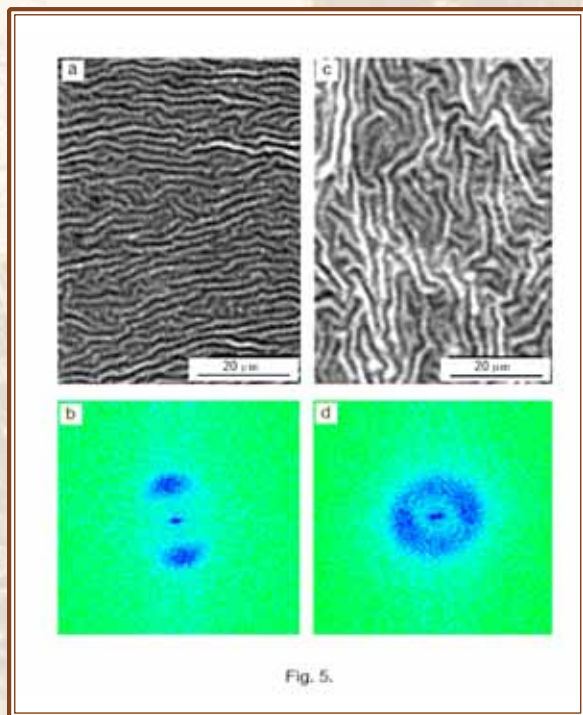


Figure 5. Domains of Marangoni regular, and chaotic roll structures: a) SEM micrograph of the regular domain; b) Fourier spectrum of regular domain in Fig.a.; c) SEM micrograph of the chaotic domain; d) Fourier spectrum of chaotic domain in Fig.c.

EDUCATION

Members of Division of Materials Physics teach 7 graduate and 3 postgraduate courses of physics and related topics at the Faculty of Sciences, Faculty of Electrical Engineering and Computing, Faculty of Chemical Engineering and Technology in Zagreb and elsewhere.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

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

Program supported by the Ministry of Sciences, Education and Sports

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

Research, developmental and international projects

1. Research of defects in Si and Ge induced by fast neutrons, Branko Pivac (Croatia-Slovenia)
2. Quantum effects in vibrational states of nanocrystalline silicon, Davor Gracin (Croatia-Slovenia)
3. Thin ZnO layer optimization in amorphous silicon PV cells, Davor Gracin, (Croatia-Macedonia)

4. Laser-induced surface self-organization: formation of surfaces with special properties, Stjepan Lugomer (Croatia-Hungary)
5. Ion beam modifications of SiC for electronic and optoelectronic applications, Branko Šantić (Croatia-Hungary)
6. Research on silicon and germanium nanostructures, Branko Pivac, (COGITO - Bilateral collaboration with France)
7. LPMAS, Davor Gracin (EU- FP6 -INCO- Project No FP6-509178)
8. The origin of structural defects and their effects upon the properties of silicate glass, Davor Gracin, (National Science Foundation of Croatia)

SELECTED ORGANIZED CONFERENCES

**15. Međunarodni sastanak
"Vakuumaska znanost i tehnika"**

Hotel Turist, Varaždin, 04.06.2008.



Organizatori:
Hrvatsko vakuumsko društvo & Društvo za vakuumsko tehniko Slovenije
www.cro-vacuum.hr/15HS2008.html

<p>Programski odbor:</p> <p>M. Jakšić M. Godec B. Pivac D. Resnik P. Pervan M. Čekada S. Milošević M. Mozetič</p>	<p>Organizacijski odbor:</p> <p>N. Radić B. Šetina H. Zorc S. Žižek M. Pavlović A. Vesel T. Car J. Kováč</p>
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The 15th International Meeting "Vacuum Science and Technique", Varaždin, June 4, 2008, was organized by the Division members N. Radić, B. Pivac, I. Capan and T. Car on behalf of the Croatian Vacuum Society. The attendance was 60 participants, and the Book of Abstracts was published.

SELECTED INVITED LECTURES

1. Armellini C, Biljanović P, Berneschi S, Bhaktha SNB, Boulard B, Chiappini A, Chiasera A, Arfuso Duverger C, Feron P, Ferrari M, Huy PT, Ivanda M, Jestin Y, Moser E, Nunzi Conti G, Pelli S, Righini GC, Speranza G. Optical properties and fabrication of glass-based erbium activated micro-nano photonic structures. MIPRO 2008, Opatija, Croatia, 26-30 May 26-30, 2008.
2. Ivanda M, Ristić D, Furić K, Musić S, Ristić M, Gotić M, Štefanić G, Crnjak Orel Z, Bitenc M, Montagna M, Ferrari M, Chiasera A, Jestin Y. Low-Frequency Raman Scattering in Materials Research, EUCMOS 2008 - XXIX European Congress on Molecular Spectroscopy, Opatija, Croatia, August 31 – September 5, 2008.

SELECTED PUBLICATIONS

1. Su DS, Xiaowei C, Xi L, Delgado JJ, Schloegl R, Gajović A. Mount-Etna-Lava-Supported Nanocarbons for Oxidative Dehydrogenation Reactions. Adv Mater 2008: 20: 3597.
2. Kukovec BM, Vaz PD, Popović Z, Calhorda MJ, Furić K, Pavlović G, Rajić Linarić M. Pseudopolymorphism in nickel(II) complexes with 6-methylpicolinate. Synthesis, structural, spectroscopic, thermal and density functional theory studies. Cryst Growth Des 2008: 8 : 3465.
3. Kuitunen K, Tuomisto F, Slotte J, Capan I. Divacancy clustering in neutron-irradiated and annealed n-type germanium. Phys Rev B 2008: 78 : 033202.
4. Žonja S, Očko M, Ivanda M, Biljanović P. Low temperature resistivity of heavily boron doped LPVCD polysilicon thin films. J Phys D: Appl Phys 2008: 41: 162002.
5. Buljan M, Bogdanović Radović I, Jakšić M, Desnica UV, Ivanda M, Saguy C, Kalish R, Djerdj I, Tonejc A, Gamulin O. Implantation conditions for diamond nanocrystals formation in amorphous silica. J Appl Phys 2008: 104: 034315.
6. Lugomer S, Geretovszky Z, Szorenyi T. Laser generation of regular wavy patterns by nonlinear instability of a metal nanolayer. J Appl Phys 2008: 104: 054911.
7. Ristić D, Ivanda M, Furić K, Desnica UV, Buljan M, Montagna M, Ferrari M, Chiasera A,

Jestin Y. Raman scattering on quadrupolar vibrational modes of spherical nanoparticles. J Appl Phys 2008: 104: 073519.

8. Maksimović A, Lugomer S, Geretovszky Z, Szorenyi T. Laser-Induced Convection Nanostructures on SiON/Si Interface. J Appl Phys 2008: 104: 124905.

CHAPTERS IN BOOKS:

1. Turković A. SAXS Characterization of Mesoporous Thin Films: A Solar Energy Point of View, Chapter 11, Solar energy: Research, Technology and Applications. Nova Science Publishers, Ed. William L. Olofsson and V.I. Bengtsson, 2008, pp 1-29.

Division of Laser and Atomic Research and Development

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

LAIR

DIVISIONAL ORGANIZATION

Head: Hrvoje Zorc

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

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



OVERVIEW OF THE DIVISION

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

The Division is currently working on several strategic projects: modelling of thin films mixtures using effective medium theories, research on plasmonic properties of metallic nanoclusters and blind and semi-blind signal processing.

TOP ACHIEVEMENTS

Optical thin films

The modelling of thin film mixtures using effective medium theories was successfully used for analysis of the refractive index of a mixture. However, the analysis of spectrophotometric

data of niobia-silica mixtures has shown that such theories fail to describe the variation of the absorption coefficient (Sancho-Parramon and Janicki, 2008). A theoretical framework, that explains the failure of these theories, in weak absorption ranges, has been developed on the basis of the spectral density function theory (Sancho-Parramon et al., 2008a). A parameterization of the compositional dependence of the parameters defining the absorption coefficient has been proposed as an alternative methodology to predict the absorption behaviour of mixtures. The characterization of novel complex coatings (rugate filters with in-depth variation of refractive index) has been reported (Janicki et al., 2008).

A new research line in thin films has been started, focused on the plasmonic properties of metal island films. This kind of films consists of a two-dimensional ensemble of nanometric metal clusters deposited on a glass substrate that can be produced by controlled evaporation of noble metals. These films show unique optical properties

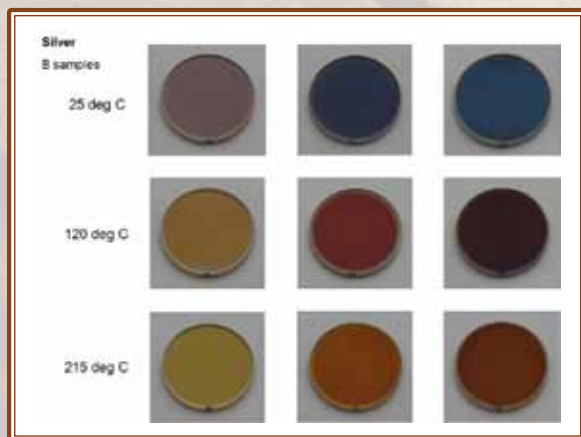


Figure 1. Tuning of optical properties of metal island films deposited on glass substrates by modification of deposition parameters.

because of the surface plasmon resonance of electrons of isolated metal clusters. By varying the deposition conditions, such as deposited thickness, substrate temperature or deposition rate, the structural and geometrical properties of the clusters can be widely varied, enabling a broad tuning of optical properties of the films (Figure 1). Structural and optical characterization of the films have been carried out using different techniques (AFM, GISAXS, ellipsometry) in the framework of international cooperation. A novel method for the dissolution of metal islands has been proposed, consisting of the application of electric field and temperature (Sancho-Parramon et al., 2008b).

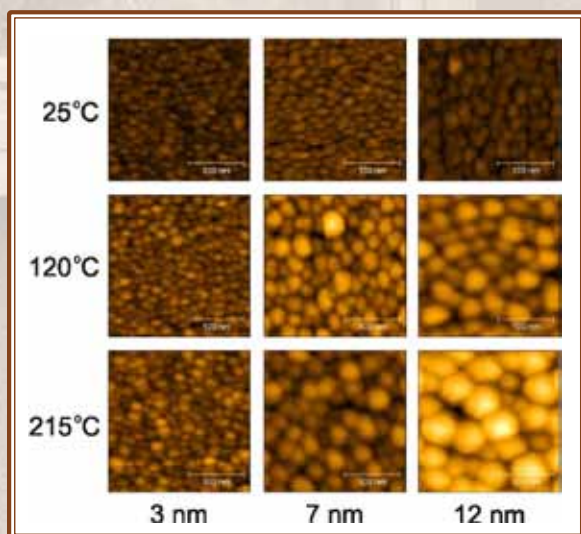


Figure 2. Nanoclusters of silver produced under various conditions.

Signal processing

The research activities have been focused on the area of blind and semi-blind signal processing: model-free blind deconvolution of temporally/spatially correlated signals, non-negative matrix factorization and sparse component analysis. Applications of the above mentioned blind signal processing methods were related to multispectral image decomposition, blind image deconvolution, compressed sensing, NMR and FT-IR spectroscopy.

EDUCATION

Members of the Division teach three courses at the Faculty of Electrical Engineering, University of Osijek, and in the Polytechnic College in Velika Gorica.

PATENTS

1. Kopriva I, Method for real time tumor visualisation and demarcation by means of photodynamic diagnosis, WO 2008/132522 A1.
2. Szu H, Buss J, Kopriva I, Nonlinear blind demixing of single pixel underlying radiation sources and digital spectrum local thermometer, US Patent 7,366,564, April 29, 2008.
3. Kopriva I, Jerić I, Smrečki V, Method of and system for blind extraction of more than two pure components out of spectroscopic or spectrometric measurements of only two mixtures by means of sparse component analysis, PCT /HR2008/000037.
4. Peršin A, Zorc H, Tisaj K, Stanišić V, Agatić N., Radman A, Soldo Roudnicky D, Lončarić M, Intelligent sequential device for photodynamic therapy, Patent P20060149

NEW EQUIPMENT

1. Digital Lock-in amplifier - Stanford research systems – SR 850.
2. Furnace - Lindberg/Bluem BS 51700

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sports

1. Analysis of multispectral data, Ivica Kopriva.
2. Optical properties of nanostructured layers, Hrvoje Zorc.

Research, developmental and international projects

1. Optical properties of metal nanoparticles embedded in dielectric multilayers, Hrvoje Zorc (International collaboration between RBI and Institute of Nanostructured Materials and Photonics, Weiz, Austria)

SELECTED INVITED LECTURES

1. Kopriva I. Blind separation of signal sources, Polytechnic of Turin, Laboratory for Engineering of the Neuromuscular Systems, May 21, 2008.

SELECTED PUBLICATIONS

1. Sancho-Parramon J, Janicki V. Effective medium theories for composite optical materials in spectral ranges of weak absorption: the case of Nb_2O_5 - SiO_2 mixtures. J Phys D: Appl Phys 2008; 21: 215304.

2. Sancho-Parramon J, Janicki V, Zorc H. Compositional dependence of absorption coefficient and band-gap for Nb_2O_5 - SiO_2 mixture thin films. Thin Solid Films 2008a; 16: 5478.
3. Janicki V, Sancho-Parramon J, Zorc H. Refractive index profile modelling of dielectric inhomogeneous coatings using effective medium theories. Thin Solid Films 2008; 10: 3368.
4. Sancho-Parramon J, Janicki V, Arbiol J, Zorc H, Peiro F. Electric field assisted dissolution of metal clusters in metal island films for photonic heterostructures. Appl Phys Lett 2008b; 16: 163108.
5. Kopriva I, Seršić D. Wavelet Packets Approach to Blind Separation of Statistically Dependent Sources, Neurocomputing, 2008; 71: 1642.
6. Du Q, Kopriva I. Automated Target Detection and Discrimination Using Constrained Kurtosis Maximization, IEEE Geoscience Remote Sensing Let 2008; 1: 38.
7. Du Q, Kopriva I. Dependent component analysis for blind restoration of images degraded by turbulent atmosphere, Neurocomputing, 2008; 10: 1016.
8. Wasylkiwskyj W, Kopriva I. Second and Fourth Order Statistics - Based Reduced Polynomial Rooting Direction Finding Algorithms, Signal Processing 2008; 10: 1016.



Division of Electronics

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

DIVISIONAL ORGANIZATION

Head: Tomislav Šmuc

The Division of electronics consists of two laboratories and one group:

- ⇒ Laboratory for information systems, Dragan Gamberger
- ⇒ Laboratory for stochastic signals and processes research, Branka Medved Rogina
- ⇒ Group for computational biology and bioinformatics, Tomislav Šmuc



ery in scientific applications” comprised from 5 related research projects, 3 of them within the Division, including a number of researchers from different faculties of the University of Zagreb and industrial partners (<http://lis.irb.hr/KDSA2008/>). Besides that, the Division works on a number of international multilateral (EU FP6 project HEARTFAID) and bilateral projects, as well as R&D projects with industry. The Division’s contribution to the higher education curriculum was extended with a graduate course on artificial intelligence at the Faculty of Science.

OVERVIEW OF THE DIVISION

The main topics of research in the Division comprise research and development of novel intelligent data and signal analysis techniques, knowledge representations for information systems, and variety of tailored applications of these techniques in biomedicine, computational biology and bioinformatics, as well as in development of advanced measurement techniques. The strong multi-disciplinary orientation is best reflected in the publication record of the Division’s members, and collaborations in multidisciplinary projects.

In 2008, the Division was granted a new research project entitled “Machine learning of predictive models in computational biology”, financed by the Croatian Ministry of Sciences, Education and Sports, for the period 2008-2011. Members of the Division organized a 2 day workshop for the research programme “Computational knowledge discov-

TOP ACHIEVEMENTS

Filtering proteomic signals

A new computational method, applied to measurements derived from chromatographic separations of biomolecular mixtures (for instance capillary or gel electrophoresis), has been developed in collaboration with the group of Krsnik-Rasol from the Department of Biology, Faculty of Science. The method involves several steps in which a larger number of measurements is processed using machine learning techniques (PCA, RF), enabling reliable determination

of relevant fractions for the particular discrimination problem, and improving computational models for class distinction based on a filtered set of relevant fractions (Figure 1).

Knowledge representation and reasoning for healthcare

The R&D efforts within the HEARTFAID project (EU6FP ICT-STREP) included the coupling of Bayesian network reasoning to the already developed ontology-based reasoner. This extension significantly enhances decision support capabilities of the system, providing reasoning in situations in which some information is missing. Besides this work, extensive analyses of the proprietary follow-up study database has been done in order to form new models for the prognosis of elderly patients suffering from heart failure syndrome.

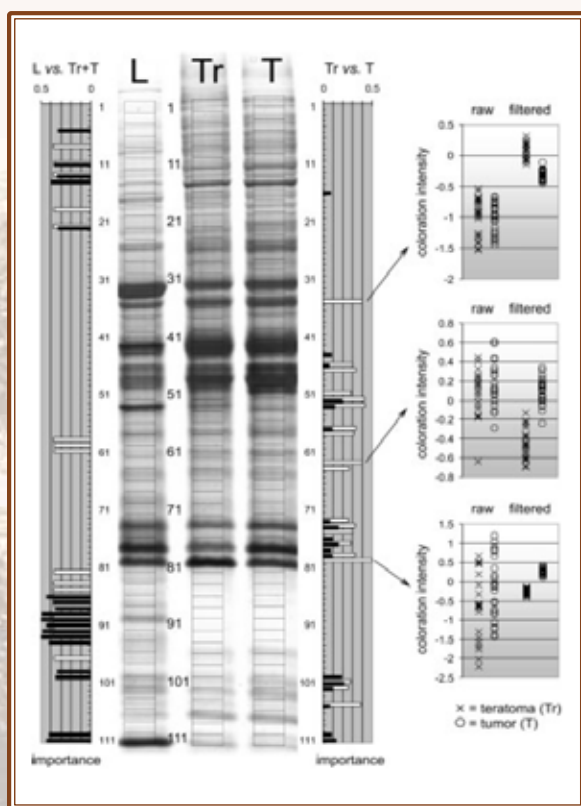


Figure 1. Extraction of most informative gel windows using novel computational method, from SDS PAGE measurements.

Finite-state data representation algorithms

An efficient method for the implementation of a sub-sequential transducer has been developed. A transducer is a finite state automaton that, on every input sequence symbol, produces a specific output symbol during transition from state to state. If the whole output sequence is associated with the final state, the transducer is called sub-sequential. Our implementation is the most efficient one regarding space requirements while preserving high speed inherent to automata structures. The applications for transducers are numerous and vary from natural language processing and human machine interface, to machine learning and data mining.

Biomedical applications

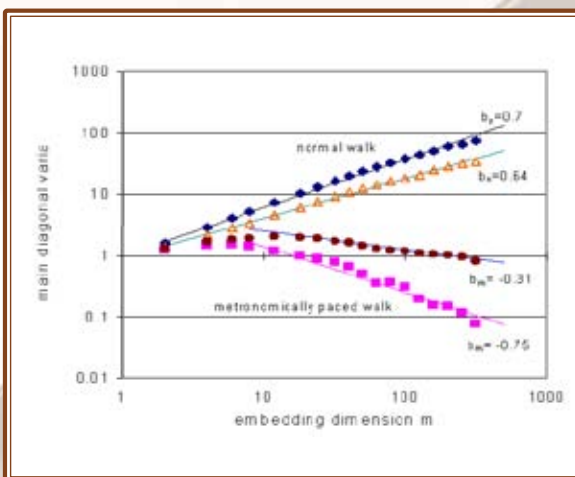


Figure 2. Scaling exponents for human gait data.

Two applications in our current research focus are related to the human walk and human jaw movement. The first method comprises the extraction of dynamic features of the human walk and the embedding of related time series data in high pseudo phase space. Subsequent projection of the embedded vectors on principal axes and/or on the main diagonal of embedding space enables extraction of fractal features from the data

(Figure 2). This research is part of our collaboration with the Faculty for Kinesiology, University of Zagreb. The second application is based on the measurements using tri-axial MEMS wireless acceleration sensor wherein accelerometric profiles of averaged vertical jaw acceleration and velocity are measured. In collaboration with the School of Dental Medicine, University of Zagreb, a study including healthy subjects without any signs or symptoms of temporomandibular disorders provides the standard profiles necessary for future studies.

Methods for the assessment of reliability of FPGA based embedded system design

A high-resolution automated measurement system for verification of timing parameters, including different methods for evaluation of metastability characteristics of programmable logic devices in industrial embedded systems, has been proposed. Three different methods, based on increased propagation delay for evaluation of metastability characteristics, were demonstrated on FPGA devices from new families of several leading manufacturers. The resolution time constant τ and the width of metastability window (W) have been determined as characteristic parameters for metastability performance of bistable devices. Using these methods it is possible to predict the metastability-induced failure rate of a device at specific (high) clock frequencies.

EDUCATION

The Division provides annually 5 courses at various faculties of the University of Zagreb.

AWARDS

Fran Supek was awarded The Croatian State Award for interdisciplinary research in the field of bioinformatics in biotechnical sciences.

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sports

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

Programs supported by the Ministry of Sciences, Education and Sports

1. Computational knowledge discovery in scientific applications, Dragan Gamberger

Research, developmental and international projects

1. HEARTFAID – A knowledge based platform of services for supporting medical-clinical management of heart failure within elderly population, Dragan Gamberger (EUFP6, ICT-STREP project)
2. Intelligent Data Analysis, Dragan Gamberger (Croatian-Slovenian bilateral project)
3. Inductive Databases for Genomics and Proteomics, Tomislav Šmuc (Croatian-Slovenian bilateral project)
4. Reliability of programmable logic devices in industrial embedded systems, Branka Medved Rogina (R&D project with the Končar Institute for Electrical Engineering)

SELECTED PUBLICATIONS

1. Supek F, Peharec P, Krsnik-Rasol M, Šmuc T: Enhanced analytical power of SDS-PAGE using machine learning algorithms. *Proteomics* 2008; 8: 28.
2. Malenica, M, Šmuc T, Šnajder J, Dalbelo Bašić B: Language Morphology Offset: Text Classification on a Croatian-English Parallel Corpus. *Inform Process Manag* 2008; 44: 325.
3. Supek F, Kralj, M, Marjanović, M, Šuman L, Šmuc T, Krizmanić I, Žinić B: Atypical cyto-

static mechanism of N-1-sulfonylcytosine derivatives determined by in vitro screening and computational analysis. Invest New Drug 2008: 26: 97.

4. Čož-Rakovac R, Šmuc T, Topić Popović N, Strunjak-Perović I, Hacmanjek M, Jadan M: Novel methods for assesing fish blood biochemical data. J Appl Ichthyol 2008: 24: 77.



Division of Physical Chemistry

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

DIVISIONAL ORGANIZATION

Head: Aleksandar Sablić

- ⇒ Laboratory for Chemical Kinetics and Atmospheric Chemistry, Branka Kovač
- ⇒ 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



strong presence of the Division in the European Research Area. Division members also contribute extensively to undergraduate and graduate education in Croatia (about 40 courses). Finally, the Division members organized traditional international conference 11th BRIJUNI CONFERENCE - Hydrogen: A universal saga (NATO Advanced Research Workshop) in 2008.

TOP ACHIVEMENTS

Mechanism of auxin interaction with auxin binding protein

OVERVIEW OF THE DIVISION

In 2008, members of the Division published nearly 50 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 was published in the highest ranking journals such as: Analytical Chemistry, Inorganic Chemistry, Journal of Organic Chemistry, Journal of Physical Chemistry A & B, Journal of Chemical Physics, ChemPhysChem, Biophysics Journal and Physical Review B. Almost half of those contributions were realized within international collaborations. The large number of fruitful international collaborations demonstrates the

Auxin Binding Protein 1 (ABP1), ubiquitous in green plants, binds auxins (plant hormones) with high specificity and affinity. In order to understand the proposed receptor function of ABP1, we carried out a detailed molecular modelling study. Molecular dynamics simulations showed that ABP1 can adopt two conformations, differing primarily in the position of C-terminus, and one of them is stabilised by the binding of an auxin molecule. A network of hydrogen-bonded water molecules, leading from the bulk water to the zinc-coordinated ligand in the ABP1 binding site, was formed in all simulations suggesting that the hydrogen-bonded water molecules may assist in protonation and deprotonation

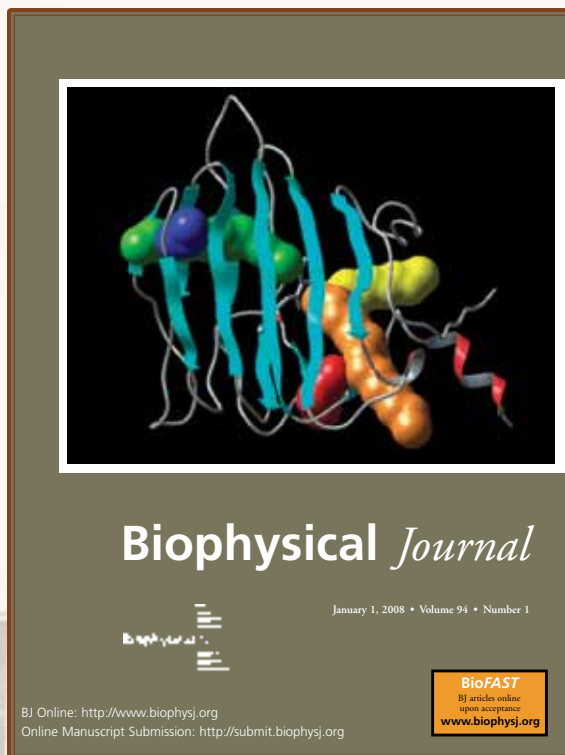


Figure 1. The front cover of *Biophysical Journal* (volume 94, issue 1) describing possible pathways used by auxin-related molecules to enter/exit their binding site in ABP1 protein (Bertoša et al., 2008).

of auxin molecules and their egress from the ABP1 binding site. Simulations of the ligand egress from ABP1 revealed three main routes by which an auxin molecule can enter or leave the ABP1 binding site (Bertoša et al., 2008). An illustration describing these results (Figure 1) appeared on the front cover of volume 94, issue 1 of *Biophysical Journal*.

Enhanced resolution for protein hydrogen/deuterium exchange

Solution-phase hydrogen/deuterium exchange, monitored by mass spectrometry, is a rapid method to study protein conformations and protein-protein interactions. Digestion efficiency for several proteins was optimized with pepsin and protease type XIII. The protease type XIII produces more fragments of shorter length and increases the signal to noise ratio, thus enhancing the sequence coverage for deuterium uptake and spatial resolution. H/D exchange for myoglobin with protease type XIII and pepsin confirms the 3-D solution structure of myoglobin by accurately locating fast- and slow-exchanging amide hydrogens in the loops and α -helices (Zhang et al., 2008).

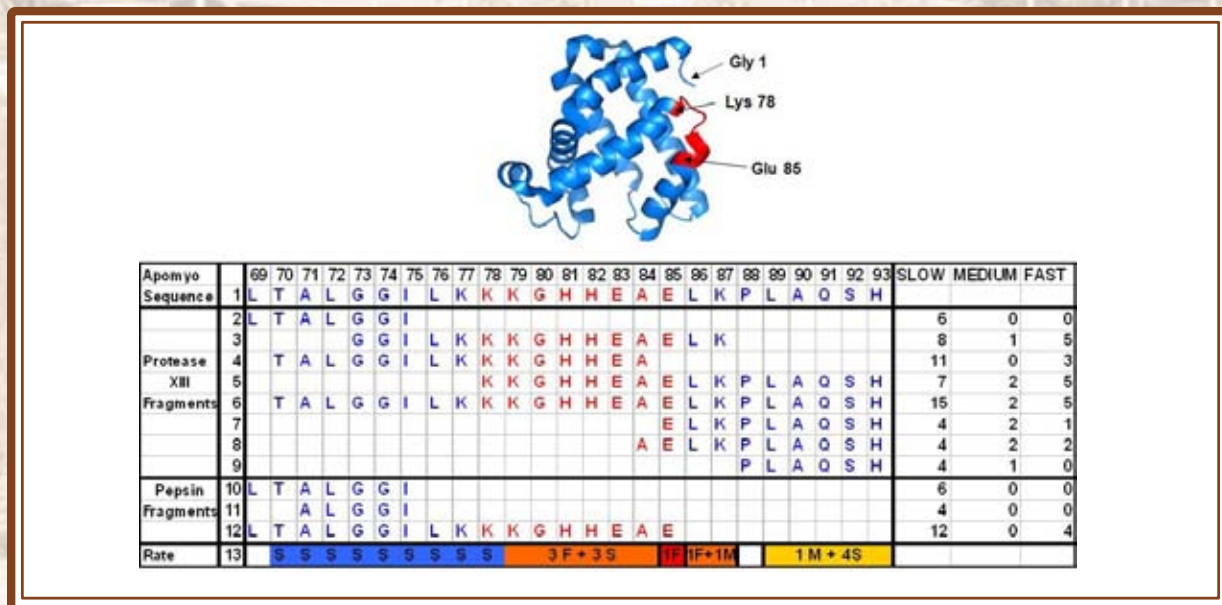


Figure 2. Exchange rates for increased sequence resolution for myoglobin segment 69-93. Amide hydrogens from the loop region 78-85 are shown in red. From the exchange rates of 11 overlapping fragments, the number of fast-, medium- and slow-exchanging hydrogens was assigned.

Electron-spin relaxation for two solid ethanol phases in the boson-peak temperature region

The approach offers the unique possibility to switch from one state of molecular packing to another within the same ethanol sample in the course of an EPR experiment. The incorporated spin probe bears information on the local dynamics and structural constraints of the glassy and crystalline environment (Kveder et al., 2008).

Double cyclopalladated complexes of azobenzenes

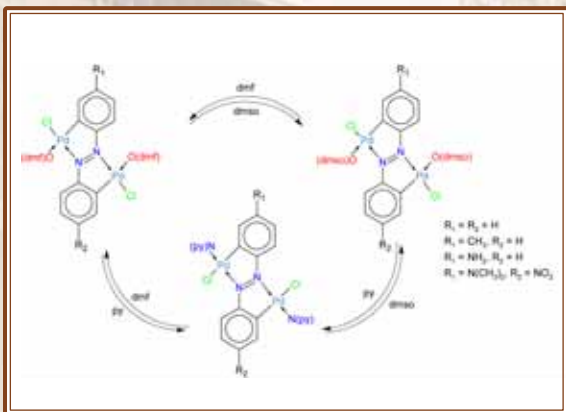


Figure 3. The solvent ligands (dmsO, dmf, py) exchange routes and cis/trans isomerization in the double cyclopalladated complexes of azobenzenes.

Since doubly cyclopalladated complexes of azobenzenes have two metalated phenyl rings, they are promising candidates for much wider application in organic synthesis, catalysis and photochemistry than their singly cyclopalladated analogues. We have prepared and characterized a new set of doubly cyclopalladated azobenzenes. Their crystal structures have been resolved and for the first time it was demonstrated that the cyclopalladation may take place at an azobenzene aromatic ring with a strong electron withdrawing substituent at the para position. The experimental results, complemented by a theoretical study, explained cis/trans isomerism in isolated complexes, their aromaticity and the nature of the electronic transitions (Babić et al., 2008).

Lipase-catalysed secondary alcohol esterification

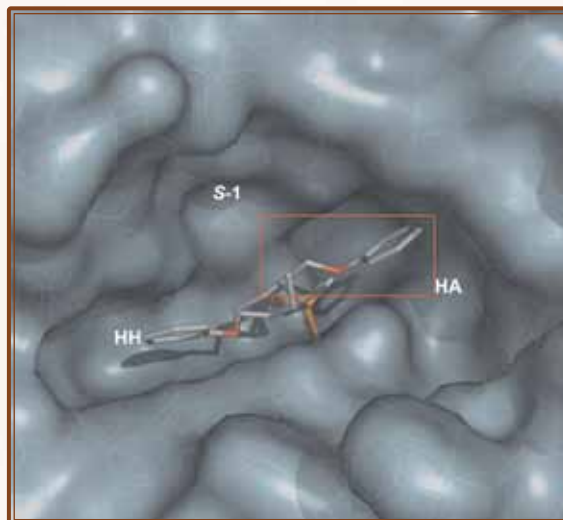


Figure 4. Comparison of binding modes of E1 ester in crystal (in red rectangular) and the one found by molecular modelling.

As a continuation of our study of the enantioselectivity towards secondary alcohols of *Burkholderia cepacia* lipase (BCL), we accomplished theoretical, MM, MC and QM/MM studies of *R*- and *S*-1-phenoxy-2-hydroxybutane-BCL complexes and determined the crystal structure of BCL complexed with a phosphonate analogue of its *S*-ester. The calculations showed that the reaction is not feasible from the crystallographically determined binding mode, but proceeds smoothly from the modelled binding mode (Luić et al., 2008).

AWARDS AND RECOGNITION

The 2008 award for young scientists and artists in the field of biology from the Society of University Teachers, Scholars and Other Scientists – Zagreb was presented to Branimir Bertoša.

EDUCATIONAL ACTIVITIES

The Division provided 21 undergraduate and 18 graduate courses at Universities in Zagreb, Split, Rijeka, Osijek and Dubrovnik.

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sport

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

Programs supported by the Ministry of Sciences, Education and Sports

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

Research, developmental and international projects

1. Chemical applications of advanced ESR-techniques, B. Rakvin (Bilateral project with Austria)
2. Application of MALDI mass spectrometry in protein and intact cell analysis: characteri-

sation of the novel SGNH-hydrolase family from *Streptomyces* and mapping of *Fusarium* parasites, I. Leščić Ašler (Bilateral project with Austria)

3. Theoretical study of the reactivity of metallo centres in proteins, S. Tomić (Bilateral project with Austria)
4. Combined experimental and theoretical study of structure and dynamics of hydrogen bonded systems, Nađa Došlić (Bilateral project with France, Program "COGITO")
5. Applications of advanced Pulsed EPR techniques in the research of new fullerene-based materials: Structural properties of Li4C60, B. Rakvin (Bilateral project with Slovenia)
6. Computer simulations of structure and dynamics of proteins, S. Tomić, (Bilateral project with Slovenia)
7. "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
8. COST physics P-15 action "Advanced Paramagnetic Resonance Methods in Molecular Biophysics", Boris Rakvin

SELECTED INVITED LECTURES

1. Rakvin B. Dynamic properties of the stable paramagnetic centres in the L-alanine crystal lattice. 6th Asia Pacific EPR/ESR Symposium, Cairns, Australia, June 13-17, 2008.
2. Živković T. A new mathematical approach for the treatment of the vibrational isotope effect. 6th Congress of the International Society for Theoretical Chemical Physics, Vancouver, Canada, July 18-27, 2008.
3. Došlić N. Multidimensional quantum dynamics of large amplitude motion. XXIX European Congress on Molecular Spectroscopy (EUCMOS-08), Opatija, August 31 – September 05, 2008.

SELECTED ORGANIZED CONFERENCES

1. 11th BRIJUNI CONFERENCE - Hydrogen: A universal saga (NATO Advanced Research Workshop), Brijuni, 25 -29 August 2008.

SELECTED PUBLICATIONS

Review articles

1. Kralj M, Tušek-Božić Lj, Frkanec L: Biomedical potentials of crown ethers: Prospective antitumor agents. *ChemMedChem* 2008: 3: 1478.

Research articles

1. Zhang H, Kazazić S, Schaub T, Tipton J, Emmett M, Marshall A: Enhanced digestion efficiency, peptide ionization efficiency, and sequence resolution for protein hydrogen/deuterium exchange monitored by FT-ICR mass spectrometry. *Anal Chem* 2008: 80: 9034.
2. Babić D, Čurić M, Molčanov K, Ilc G, Plavec J: Synthesis and characterization of dicyclopalladated complexes of azobenzene derivatives by experimental and computational methods. *Inorg Chem* 2008: 47: 10446.
3. Luić M, Štefanić Z, Ceilinger I, Hodošček M, Janežić D, Lenac T, Leščić Ašler I, Šepac D, Tomić S: Combined X-Ray Diffraction and QM/MM Study of the Burkholderia cepacia Lipase-Catalyzed Secondary Alcohol Esterification. *J Phys Chem B* 2008: 112: 4876.
4. Bertoša B, Kojić-Prodić B, Wade R, Tomić S: Mechanism of Auxin Interaction with Auxin Binding Protein (ABP1): A Molecular Dynamics Simulation Study. *Biophys J* 2008: 94: 27.
5. Vujasinović I, Veljković J, Molčanov K, Kojić-Prodić B, Mlinarić-Majerski K: Thiamacrocylic lactones: New Ag(I)-ionophores. *J Org Chem* 2008: 73: 9221.
6. Cambré S, Wenseleers W, Čulin J, Van Doorslaer S, Fonseca A, Nagy JB, Goovaerts E: Characterisation of nanohybrids of porphyrins with metallic and semiconducting carbon nanotubes by electron paramagnetic resonance and optical spectroscopy. *ChemPhysChem* 2008: 9: 1930.
7. Kveder M, Merunka D, Jokić M, Rakvin B: Electron-spin relaxation in crystalline and glassy state of solid ethanol in the boson-peak temperature region. *Phys Rev B* 2008: 77: 094202.
8. Matanović I, Došlić N, Johnson B: Generalized approximation to the reaction path: the formic acid dimer case. *J Chem Phys* 2008: 128: 084103-1-084103-10.
9. Makong O, Flyunt R, Tobien T, Naumov S, Bonifačić M: Dimethylselenide as a probe for reactions of halogenated alkoxy radicals in aqueous solution. Degradation of dichloro- and dibromomethane. *J Phys Chem A* 2008: 112: 5916.
10. Friščić T, Klasinc L, Kovač B, MacGillivray L: HeI photoelectron spectra and gas-phase electronic structures of end-functionalized [3]- and [5]-ladderanes. *J Phys Chem A* 2008: 112: 1493.
11. Novak I, Kovač B: Electronic structure of substituted benzoquinones and quinonechloroimides. *J Phys Chem A* 2008: 112: 3061.
12. Alberti A, Galasso V, Kovač B, Modelli A, Pichierri A: Probing the molecular and electronic structure of capsaicin: A spectroscopic and quantum mechanical study. *J Phys Chem A* 2008: 112: 5700.
13. Galasso V, Kovač B, Modelli A, Ottaviani MF, Pichierri F: Spectroscopic and theoretical study of the electronic structure of curcumin and related fragment molecules. *J Phys Chem A* 2008: 112: 2331.



Division of Organic Chemistry and Biochemistry

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

ZOKB

DIVISIONAL ORGANIZATION

Head: Mirjana Eckert-Maksić till June, Kata Majerski

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

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



organic chemistry; stereoselective synthesis and catalysis; supramolecular chemistry, including gels, and host-guest interactions; interactions of small molecules with DNA/RNA, chemistry of peptides, glycopeptides and peptidomimetics; molecular spectroscopy; experimental and computational protein biochemistry and molecular enzymology, and quantum organic chemistry.

The results of the work are published in 59 scientific papers, which appeared mostly in high ranking chemical journals. In addition, 5 patent applications were submitted.

Members of the Division have made significant contributions to higher education by providing courses at undergraduate and doctoral level and by supervising B. Sc. (6) M.Sc. (1) and Ph.D. (2) thesis. They are also active in national and international societies and bodies and serve as the editors or the members of several editorial boards.

OVERVIEW OF THE DIVISION

The excellence in scientific research was maintained in the Division throughout 2008. The majority of the work effort was devoted to the basic research in the fields of organic and bioorganic chemistry. There were several important discoveries in a broad range of topics such as synthetic and physical or-

TOP ACHIEVEMENTS

The first structure of dipeptidyl peptidase III

Figure 1. Structure of the *Saccharomyces cerevisiae* DPP III enzyme. The catalytic zinc ion is shown in yellow.

Dipeptidyl peptidase III (DPP III) is a zinc-dependent enzyme with an implied role in the pain-modulatory system and endogenous defence against oxidative stress in mammals. Two members of the DPP III family were studied in parallel. For the human orthologue, a functional role of Tyr318 was predicted based on the mutagenesis approach, which resulted in a publication in Biological Chemistry. Yeast DPP III was cloned, heterologously expressed and the 1.95-Å crystal structure was resolved, representing the prototype for the whole family (Figure 1). It shows a novel protein fold and provides insight into the catalytic mechanism and mode of substrate binding. The yeast enzyme shows a high degree of conservation to mammalian DPP III in the active site and thus provides the basis for rational drug design (Baral et al., 2008).

The latter article was selected as a Paper of the Week in the Journal of Biological Chemistry (JBC) and was also included in a cumulative collection of JBC Papers of the Week.

Interactions of novel benzimidazole derivatives with DNA/RNA and biological activity

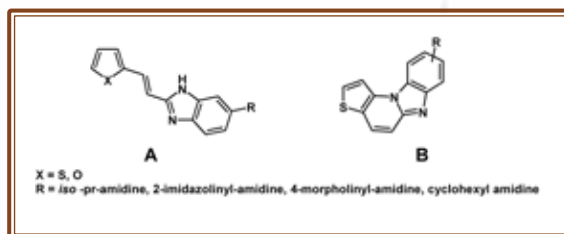


Figure 2. General structures of studied benzimidazole derivatives.

Detailed studies of the interactions between novel “non-fused” benzimidazole derivatives (Figure 2A) and their “fused” analogues (Figure 2B) with natural and synthetic double stranded DNA and RNA unambiguously revealed that the “non-fused” derivatives (A) bind into DNA minor groove, while their “fused” analogues (B) intercalate in both, DNA and RNA. Different *in vitro* antitumor activity mechanisms of “non-fused” and “fused” derivatives were directly correlated to the DNA binding modes of studied compounds (Hranjec et al., 2008)

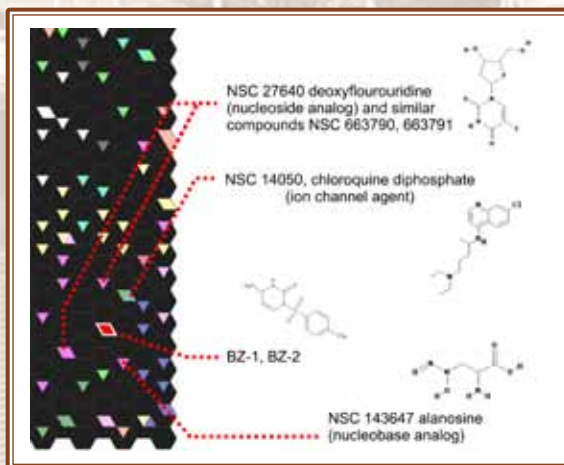
Atypical cytostatic mechanism of *N*-1-sulfonylcytosine derivatives

Figure 3. A self-organizing map constructed using i2SOM software contains 537 compounds belonging to one of 12 mechanistic classes plus the two BZ compounds.

N-1-Sulfonylpyrimidine derivatives have strong antiproliferative activity, whereby 1-(*p*-

toluenesulfonyl)cytosine, BZ-1 showed a selective effect to normal cells. Supervised machine learning methodology (Random Forest classifier) was used for analysis of cytostatic activity profiles (Figure 3). The computational results, taken together with cell cycle perturbation and apoptosis analysis, point to an unusual mechanism of cytostatic action, possibly a combination of nucleic acid antimetabolite activity and a novel molecular mechanism (Supek et al., 2008).

Domino photochemistry of N-(1-adamantyl)phthalimide

The photochemical reaction of N-(1-adamantyl)phthalimide (Figure 4) yields the novel hexacyclic benzazepine derivative of 2,4-methanoadamantane (2), as a clean single product. Its structure, characterized by X-ray analysis, represents the first example of the 2-azahehexacyclo[8.7.1.1^{11,4}.0^{4,9}.0^{11,16}.0^{12,18}]nonadeca-4,6,8-triene skeleton. The product is formed by a domino process of two consecutive excited state intramolecular hydrogen transfer reactions. Base hydrolysis of the benzazepine (2) gives the keto derivative of the 1,2-substituted adamantane ϵ -amino acid (3) in high yield (Basarić et al., 2008).

Epoxides to chiral oxazolidinones

Halohydrin dehalogenase from *Agrobacterium radiobacter* catalyzed the enantioselective ring opening of terminal epoxides with cyanate as a nucleophile, yielding 5-substi-

tuted oxazolidinones in high yields and with high enantiopurity (69-98% ee). This is the first example of the biocatalytic conversion of a range of epoxides to the corresponding oxazolidinones (Majerić Elenkov et al., 2008).

Hydrogen bonding in 1,1'-bi-2-naphthol within the polarizable continuum model

The intra- and intermolecular hydrogen bonding of 1,1'-bi-2-naphthol in a series of solvents and in the solid phase has been investigated by means of mid-IR spectroscopy and DFT reaction-field calculations. The results show that the relative stability of isomers, differing in the positions of the hydroxyl groups, are the same in hydrogen-bond non-accepting solvents and the gas phase, although the less stable isomers are more probable in solvents of higher relative permittivity. In hydrogen-bond forming solvents, the least stable isomer is most probably prevalent due to the additional stabilization through intermolecular hydrogen bonds with solvent molecules. A detailed vibrational analysis revealed the spectral regions specific to the OH vibrations with the observed solvent effects concerning the redistribution of vibrational intensities rather than wave-number shifts (Biliškov et al., 2008).

Surface-enhanced Raman scattering on colloid gels

Surface-enhanced Raman scattering (SERS) has been applied to study weak in-

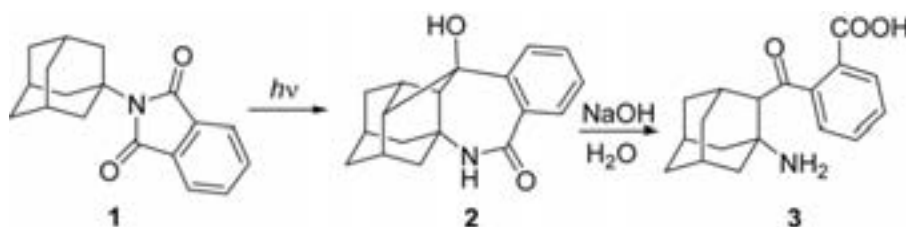


Figure 4. Domino photochemistry of 1.

termolecular interactions between small organic gelling molecules involved in the silver and gold nanoparticle-hydrogel composite formation. Strong Raman signals dominate in SERS spectra of hydrogels containing silver nanoparticles prepared by the citrate and borohydride reduction methods, whereas broad bands of low intensity are detected in the spectra of gold colloid gels. Transmission electron microscopy reveals a dense gel structure in the close vicinity of the enhancing metal particles for both silver colloid gels (Miljanić et al., 2008).

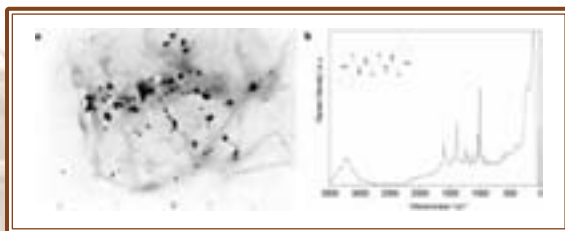


Figure 5. (a) TEM images of silver citrate colloid hydrogel of bis(S-phenylalanine)oxalyl amide, magnification 25 000 x and (b) its SERS spectrum.

New Ag(I)-ionophores

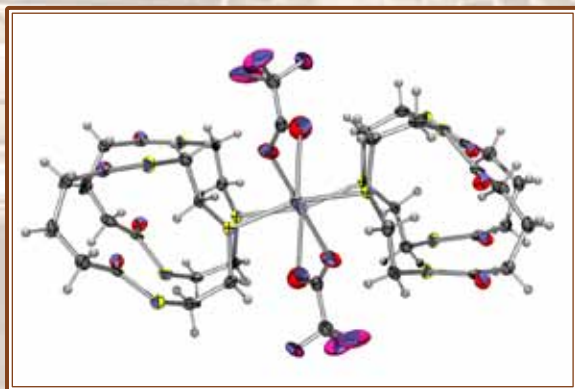


Figure 6. Ball-and-stick representation of [4:2] silver complex with thialactone ligand $\text{Ag}(13)_2$ determined by X-ray structure analysis.

New macrocyclic hosts, varying in size of macrocyclic ring, the number of flexible or adamantane moieties and the number of donor atoms, were prepared, and their complexing ability toward transition and heavy metal cations (Ag^+ , Cu^{2+} , Zn^{2+} , Cd^{2+} , Pb^{2+}) was studied. In picrate extraction surveys, it was possible to show that most of the hosts studied are good Ag^+ acceptors. The structural analysis of

complexes $\text{Ag}13$ and $\text{Ag}(13)_2$ (Figure 6) suggest that preferred ambidentate tetracoordination of Ag^+ ions is favourable for the molecules with flexible rings (Vujasinović et al., 2008).

Successful characterization of mixed-ligand Fe(II) complexes

Formation of novel mixed-ligand iron complexes, containing 1,10-phenanthroline, 1,10-phenanthroline-5,6-dione, and NCS^- as ligands, were analyzed by electrospray ionization ion trap MS/MS. Under the applied electrospray ionization mass spectrometry (ESI-MS) conditions, MeOH, water, and EtOH formed solvent clusters around the free or complexed 1,10-phenanthroline-5,6-dione. Owing to the solvent-ligand hydrogen-bond formation, the solvent-ligand clusters were formed in the polar protic solvents. The number of protic solvent molecules per complex ion in cluster depended on the number of 1,10-phenanthroline-5,6-dione ligands in the complex ion. Unlike MeOH, EtOH, or water, ACN was not involved in the formation of the solvent clusters with the iron complexes containing 1,10-phenanthroline-5,6-dione as ligand (Kobetić et al., 2008).

Guanidinium ions separated by para-phenylene spacer

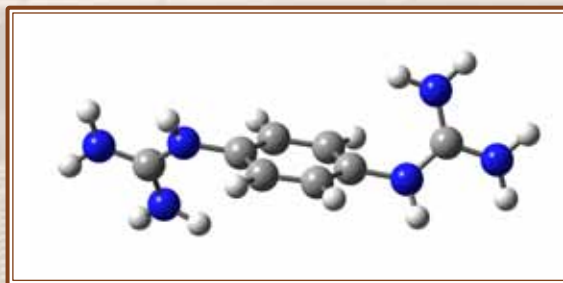


Figure 7. Schematic presentation of the optimized structure of double protonated para-bisguanidylbenzene dication.

The stability and fragmentation mechanism of the mono- and the doubly protonated guanidinium ions, generated via electrospray ionization of para-bisguanidylbenzene and its permethylated derivatives, were investigated and rationalized using

DFT calculations. The obtained dications are the first examples of multiply charged cations of this type generated in the gas phase (Tintaru et al., 2008).

Reactivity and oxidative potential of sugars in peptide-sugar model systems

Fructose is a sugar that participates in the formation of toxic advanced glycation products, which appear to play a role in the pathogenesis of the vascular, renal and ocular complications of diabetes. The reactivities of fructose and glucose in model systems containing bioactive peptides (enkephalins) were compared. The obtained results indicate that glucose is more reactive than fructose, with respect to the formation of *N*-glycated peptides. However, fructose has the higher oxidative potential to damage methionine residues in peptides (Jakas et al., 2008).

Novel chloroenyne-modified amino acid derivatives

Naturally occurring enediyne compounds are among the most effective anticancer agents known, and synthetically modified enediynes are lead chemotherapeutics today. Three groups of chloroenyne-modified amino acids carrying different protecting groups were synthesized. The optimal conditions for the coupling of amino acid-derived acetylenes with alkenyl chlorides were described and elucidated (Gredičak et al., 2008).

Superacids: How far can one go?

Computational studies of neutral organic superacids were continued and the most powerful hyperacid was designed by using polycyanated extended molecular framework of Rees' annulenes. The manuscript describing the results was published in the New Journal of Chemistry, where it was selected as a "hot article".

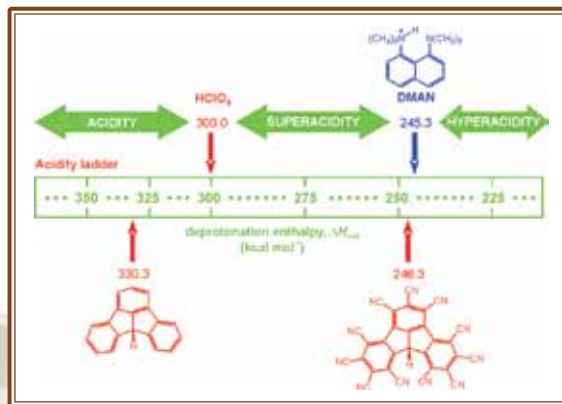


Figure 8. Undecacyanofluoradene is the first neutral hyperacid as predicted by computational chemistry.

Patent applications

Patent Application WO2008102127 (A3), Čaplar V, Frkanec L, Jokić M, Makarević K, Portada T, Žinić M, Jelčić Ž. (Pliva Hrvatska d.o.o.), Gel forming compounds.

Patent Application WO2008113992 (A3), Čaplar V, Frkanec L, Jokić M, Makarević K, Portada T, Žinić M, Jelčić Ž. (Pliva Hrvatska d.o.o.), Gel compositions.

Patent Application WO2008/114067 (A1), Basarić N, Renić M, Mlinarić-Majerski K. Adamantane-dipyrromethane derivatives, method of preparation and applications in anion sensing.

Patent number P2080102A, Landek G, Kontrec D, Vinković V. New Chiral Stationary Phases for Chromatography Based on Aromatic Allyl Amines.

Patent number PCT/HR2008/000037, Kopriva I, Jerić I, Smrečki V. Method of and system for blind extraction of more than two pure components out of spectroscopic and spectrometric measurements of only two mixtures by means of sparse component analysis.

New equipment

The high-pressure liquid chromatography-mass spectrometry (HPLC-MS) instrument (Agilent Technologies) was purchased with the financial help of the Ministry of Sciences, Education and Sports of the Republic of Croatia.

The acquisition of a HPLC-MS-MS instrument will contribute to the achievement of the scientific objectives in Division and open possibilities for introducing new methods and scientific fields.

EDUCATION

The Division provides annually over 27 undergraduate and graduate courses at Universities Zagreb, Osijek and Dubrovnik.

AWARDS AND RECOGNITION

David Smith: Leopold Ružička award for young scientists of the Croatian Chemical Society.

Ina Nemet, Juvenile Diabetes Research Foundation Postdoctoral Fellowship Award, "Novel Pathways of Glycation Damage in Diabetic Complications" (2008-2010).

Borislav Kovačević: Postdoctoral Fellowship from the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia: "Computational Investigation of the Biological Mechanism of Glycerol Dehydration" (1.11.2007-30.10.2008).

Danijela Barić: Postdoctoral Fellowship from the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia: "Computational Investigation of the Coenzyme B₁₂-Dependent Fermentation of Diols" (15.02-15.08.2008).

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Sciences, Education and Sports

1. Molecular enzymology and protein interactions of hydrolases, Marija Abramić
2. Macrocyclic ligands, structures in solutions and molecular spectroscopies, Goran Baranović
3. Organic and bioorganic processes in ground and excited states, Mirjana Eckert-Maksić
4. Chiral building blocks for biologically active

molecules. Synthesis and reactivity, Zdenko Hameršak

5. Chemical transformations of natural compounds, Štefica Horvat
6. Cage compounds: Building blocks for molecular architecture, Kata Majerski
7. Brønsted and Lewis acids and bases in chemistry and biochemistry, Zvonimir Maksić
8. Host-guest interactions in polycyclic systems, Davor Margetić
9. Design, synthesis and study of interactions of small molecules with DNA, RNA and proteins, Ivo Piantanida
10. Computational studies of protein structure and function, David Smith
11. Chiral organic materials - synthetic, structural and functional research, Vladimir Vinković
12. Synthesis of novel biologically active nucleobase and nucleotide derivatives, Biserka Žinić
13. Supramolecular chemistry of gels. Self-assembly approach to functional hybrid materials, Mladen Žinić

Programs supported by the Ministry of Sciences, Education and Sports

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

Research, developmental and international projects

1. Reinforcement of the Centre for Computational Solutions in the Life Sciences, David Smith (6th Framework Programme, EU-FP6-043749-ReCompSoLS)
2. Computational prediction of structure and catalytic activity of new organic superacids, Unity through Knowledge Fund project for young researchers and professionals under the call "My First Research Topic" Grant co-financed by the APO Environmental Protection Services Ltd. Zagreb, Robert Vianello
3. Artificial Receptors for Bacillus anthracis Specific Anthrose Detection, Andreja Jakas, Nato Science for Peace and Security Programme; CBP.EAP.SFP.983154
4. Photodynamical simulation of bioorganic processes, Mirjana Eckert-Maksić (Croatian-Austrian bilateral project)

5. The amide linkage and its implications in molecular biology, Robert Vianello (Croatian-Austrian bilateral project)
6. Protein engineering of halohydrin dehalogenases for the production of fine chemicals and pharmaceutical intermediates, Maja Majerić Elenkov (Croatian-Chinese bilateral project, 2007-2009)
7. Microheterogeneity in Aqueous Mixtures: An Investigation by Molecular Spectroscopy and Theoretical Methods, Goran Baranović (Croatian-French program "Cogito")
8. New functional dendritic materials: synthesis and self-organization, Andreja Lesac (Croatian-French program "Cogito")
9. Photochemical transformation of adamantane derivatives activated by phthalimides, Nikola Basarić (Croatian-German bilateral project)
10. Experimental and Computational Study of Protonated Organic Molecules, Mirjana Eckert-Maksić (Croatian-German bilateral project)
11. Computer-assisted Design of Strong and Ultra-strong Bases and their Applications, Zvonimir Maksić (Croatian-German bilateral project)
12. Metal-binding ability of Leu-enkephalin, related glycoconjugates and peptidomimetics: comparative CD and FTIR spectroscopic studies, Andreja Jakas (Croatian-Hungarian bilateral project)
13. Pores and Channels by Assembly of Cyclic Peptides: Design, Molecular Modelling and Synthesis, Kata Majerski (Croatian-Indian bilateral project)
14. Theoretical Study of Bioactive Molecules with Property of Releasing Nitrogen Monoxide (NO): N-nitrosohydroxylamine and its N- and O- alkyl Derivatives, Mirjana Eckert-Maksić (Croatian-Slovenian bilateral project)
15. Theoretical and Experimental Investigations of the Intra- and Intermolecular Hydrogen Bonds, Zvonimir Maksić (Croatian-Slovenian bilateral project)
16. Thermally processed foods: possible health implication, Štefica Horvat and Andreja Jakas (COST 927, WG1 and WG5)
17. Organising Non-Covalent Chemical Systems with Selected Functions, Mladen Žinić (COST D31)
18. Design, synthesis and molecular interactions of bis-porphyrin molecular receptors, Croatian Academy of Arts and Sciences, Davor Margetić
19. Polyfunctional guanidines. Design, synthesis and catalytic properties of novel superbas-

es, Croatian Academy of Arts and Sciences, Zoran Glasovac

SELECTED INVITED LECTURES

1. Basarić N: Domino photochemistry of adamantane phthalimides, Central European Conference on Photochemistry, Bad Hofgastein, Austria, February 10-14, 2008.
2. Maksić ZB: Acidity and basicity in solutions – a selection of the best model and implication for grid applications, COST D37 meeting, Barcelona, Spain, May 22–23, 2008.
3. Smith DM: Computational Investigations of Enzyme Mechanisms: An Application to the Dehydration of 1,2-Diols, From Solid State to BioPhysics, Cavtat, Croatia, June 06-13, 2008
4. Smith DM: Computational Investigation of Enzyme Mechanisms: An Application to the B12-Independent Glycerol Dehydratase, Trends in Enzymology, Saint Malo, France, July 02-05, 2008.
5. Maksić ZB: From concepts to computations and vice versa, Electron Correlation and Molecular Dynamics for Excited States and Photochemistry, Wien, Austria, July 03–04, 2008
6. Majerski K: Influence of the rigid spacer to macrocyclization of poly(thialactones): synthesis and computational analysis, 19th IUPAC Conference on Physical Organic Chemistry, Santiago de Compostela, Spain, July 13–18, 2008.
7. Eckert-Maksić M: Dynamics simulations of photodissociation of formamide and its protonated form in the gas phase, 19th IUPAC Conference on Physical Organic Chemistry, Santiago de Compostela, Spain, July 13–18, 2008
8. Maksić ZB: Acidity and basicity of 20+2 α -amino acids in vacuo and water solutions, 19th IUPAC conference on physical organic chemistry, Santiago de Compostela, Spain, July 13–18, 2008.
9. Maksić ZB: Design of organic superacids and superbases "ex machina" – an interplay between conceptual and computational chemistry, 7th European Conference on Computational Chemistry, Venice, Italy, September 11–15, 2008.
10. Smith DM: A Computational Investigation of Enzyme Mechanisms: An Application to the Dehydration of 1,2-Diols, The Eighth Triennial Congress of the World Association of

Theoretical and Computational Chemists (WATOC 08), Sydney, Australia, September 14-19, 2008.

11. Smith DM: Computational Investigations of the Mechanism of Enzyme Action: An Application to the Dehydration of 1,2-Diols, The International Conference on the Theory and Applications of Computational Chemistry in 2008 (TACC2008), Shanghai, China, September 23-27, 2008.
 12. Eckert-Maksić M: Photodissociation of formamide and its protonated forms – An *ab initio* surface hopping dynamics simulations, The Centre for Computational Chemistry, University of Georgia, Athens, USA, September 25, 2008.
 13. Maksić ZB: From concepts to computations and back – design of strong organic superacids and superbases, Twenty second annual Charles A. Coulson lecture, University of Georgia, Athens, Georgia, U.S.A., September 30, 2008.
 14. Vianello R: Extremely acidic neutral organic superacids – computationally predicted molecules awaiting experimental synthesis, Workshop on new materials in industry & medicine, Zagreb, Croatia, November 25–26, 2008.
5. Majerić Elenkov M, Tang L, Hauer B, Janssen BD: Formation of enantiopure 5-substituted oxazolidinones through enzyme-catalysed resolution of epoxides. *Org Lett* 2008: 10: 2417.
 6. Biliškov N, Baranović G: Hydrogen Bonding in 1,1'-Bi-2-naphthol within the Polarizable Continuum Model, *J Phys Chem B* 2008: 112: 10638.
 7. Vujasinović I, Veljković J, Molčanov K, Kojić-Prodić B, Mlinarić-Majerski K: Thiamacrocylic Lactones: New Ag(I)-Ionophores. *J Org Chem* 2008: 73: 9221.
 8. Miljanić S, Frkanec L, Biljan T, Meić Z, Žinić M: Surface-Enhanced Raman Scattering on Colloid Gels Originated from Low Molecular Weight Gelator, *J Raman Spectrosc* 2008: 39: 1799.
 9. Kobetić R, Gembarovski D, Baranović G, Gabelica V: ESI-MS studies of mixed-ligand Fe(II) complexes containing 1,10-phenanthroline and 1,10-phenanthroline-5,6-dione as ligands. *J Mass Spectrom* 2008: 43: 753.
 10. Tintaru A, Roithová J, Schröder D, Charles L, Jušinski I, Glasovac Z, Eckert-Maksić M: Generation and Dissociation Pathways of Singly and Doubly Protonated Bisguanidines in the Gas Phase. *J Phys Chem A* 2008: 112: 12097.

SELECTED PUBLICATIONS

1. Sandala GM, Smith DM, Radom L: The Carbon-Skeleton Rearrangement in Tropane Alkaloid Biosynthesis. *J Am Chem Soc* 2008: 130: 10684.
2. Baral PK, Jajčanin-Jozić N, Deller S, Macheroux P, Abramić M, Gruber K: The first structure of dipeptidyl-peptidase III provides insight into the catalytic mechanism and mode of substrate binding. *J Biol Chem* 2008: 283: 22316.
3. Hranjec M, Piantanida I, Kralj M, Šuman L, Pavelić K, Karminski-Zamola G: Novel amidino-substituted thienyl- and furyl-vinyl-benzimidazole derivatives and their photochemical conversion into corresponding diaza-cyclopenta[c]fluorenes. Synthesis, interactions with DNA and RNA and antitumor evaluation. Part 4. *J Med Chem* 2008: 51: 4899.
4. Basarić N, Horvat M, Mlinarić-Majerski K, Zimmermann E, Neudörfl J, Griesbeck AG: Novel 2,4-Methanoadamantane-Benzazepine by a Domino Photochemistry of N-(1-adamantyl)phthalimide. *Org Lett* 2008: 18: 3965.
5. Majerić Elenkov M, Tang L, Hauer B, Janssen BD: Formation of enantiopure 5-substituted oxazolidinones through enzyme-catalysed resolution of epoxides. *Org Lett* 2008: 10: 2417.
6. Biliškov N, Baranović G: Hydrogen Bonding in 1,1'-Bi-2-naphthol within the Polarizable Continuum Model, *J Phys Chem B* 2008: 112: 10638.
7. Vujasinović I, Veljković J, Molčanov K, Kojić-Prodić B, Mlinarić-Majerski K: Thiamacrocylic Lactones: New Ag(I)-Ionophores. *J Org Chem* 2008: 73: 9221.
8. Miljanić S, Frkanec L, Biljan T, Meić Z, Žinić M: Surface-Enhanced Raman Scattering on Colloid Gels Originated from Low Molecular Weight Gelator, *J Raman Spectrosc* 2008: 39: 1799.
9. Kobetić R, Gembarovski D, Baranović G, Gabelica V: ESI-MS studies of mixed-ligand Fe(II) complexes containing 1,10-phenanthroline and 1,10-phenanthroline-5,6-dione as ligands. *J Mass Spectrom* 2008: 43: 753.
10. Tintaru A, Roithová J, Schröder D, Charles L, Jušinski I, Glasovac Z, Eckert-Maksić M: Generation and Dissociation Pathways of Singly and Doubly Protonated Bisguanidines in the Gas Phase. *J Phys Chem A* 2008: 112: 12097.
11. Eckert-Maksić M, Glasovac Z, Trošelj P, Kütt A, Rodima T, Koppel I, and Koppel IA: Basicity of Guanidines with Heteroalkyl Side Chains in Acetonitrile. *Eur J Org Chem* 2008: 5176.
12. Supek F, Kralj M, Marjanović M, Šuman L, Šmuc T, Krizmanić I, Žinić B: Atypical cytostatic mechanism of N-1-sulfonylcytosine derivatives determined by *in vitro* screening and computational analysis. *Invest New Drugs* 2008: 26: 97.
13. Gredičak M, Kolonić A, Jerić I: Novel chloroene-modified amino acid derivatives. *Amino Acids* 2008: 35: 185.
14. Jakas A, Horvat Š: Reactivity and oxidative potential of fructose and glucose in enkephalin-sugar model systems. *Amino Acids* 2008: 34: 329.
15. Vianello R, Maksić ZB: Rees polycyanated hydrocarbons and related compounds are extremely powerful Brønsted superacids in the gas-phase and DMSO – a density functional B3LYP study. *New J Chem* 2008: 32: 413.

CHAPTERS IN BOOKS

1. Roje M, Portada T: Three-membered Rings with Two Oxygen and/or Sulfur Atoms. In: Comprehensive heterocyclic chemistry III. Editor: Katritzky A. Oxford : Elsevier, 2008. pp. 641-678.
2. Monnier VM, Sell DR, Dai Z, Nemet I, Collard F, Zhang J: The role of the Amadori product in the complications of diabetes. In The Maillard Reaction: Recent Advances in Food and Biomedical Sciences. Editors: Schleicher E, Somoza V, Schieberle P. New York : Blackwell Publishing, 2008, pp 81-88.

ZOKB



DIVISIONAL ORGANISATION

Head: Svetozar Musić

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

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



unit in Croatia which covers all aspects of the physico-chemical effects of ionizing radiations and their applications. The low-dose and high-dose chemical dosimetry systems were developed and received international recognition. Our main research activities are financially sponsored by the Ministry of Sciences, Education and Sports. There are also numerous cooperations with industries, hospitals, state institutions and faculties.

TOP ACHIEVEMENTS

New method in the synthesis of nanosized iron oxides

The new synthesis of nanosized iron oxide particles by using a solvothermal approach with the participation of an esterification reaction in the iron(III)/acetic acid/alcohol system was developed. When basic iron(III) acetate was autoclaved in pure ethanol, nanosized magnetite particles were exclusively formed. In the presence of pure octanol, magnetite and some of the hematite phase was obtained. In the presence of ethanol and free acetic acid, exclusively nanosized hematite particles were obtained (Gotić and Musić, 2008).

OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is a centre of excellence in materials science. We are investigating chemical, microstructural and physical properties of various materials. Also, we are developing new methods of materials synthesis. Our primary interests are in metal oxides, glass-ceramics, zeolites, polynuclear and metal cluster compounds, organic polymers, intermetallic compounds and metal hydrides. There is a long tradition in the investigation of the kinetics and mechanisms in different precipitation systems. The radiation chemistry and dosimetry laboratory at the division is the only existing

Precipitation of calcium carbonate

Different soluble polysaccharides: cationic, anionic and non-ionic dextrans and soluble starch have been used as additives in the precipitation system of calcium carbonates. The study investigated the role of ionic charge, molecular masses and concentration of selected polysaccharides on the size distribution, morphology and mineralogical composition of precipitate. In addition, some general conclusions on the mode of substrate / macromolecule interactions in electrolyte solutions were made (Kontrec et al., 2008).

Study of microstructure of amorphous aluminosilicate gel before and after its hydrothermal treatment

Analyses of freshly prepared sodium aluminosilicate hydrogel as well as during its hydrothermal treatment at 353 K by different methods have shown that the freshly prepared gel is mainly composed of disc-shaped primary particles, but also partially or even fully crystalline entities. To arrive at this conclusion, techniques such as powder X-ray diffraction, Fourier transform infrared spectroscopy, Differential thermal gravimetry, High-resolution transmission electron microscopy and Atomic force microscopy, were used. Atomic force microscopy analysis of the solids separated from the hydrogel at various stages of its hy-



Figure 1. AFM image of the features appearing in the solid phase of the reaction mixture (initially aluminosilicate hydrogel) during its hydrothermal treatment at 80 °C for (A) 30 min ("pyramidal-shaped" particles which represent the first visualization of zeolite nuclei), (B) 90 min (zeolite A microcrystals formed by the growth of nuclei: top of nucleus can be observed near the centre of the 001 crystal faces of each microcrystal) and (C) 240 min (final product; zeolite A crystals with typical growing terraces).

drothermal treatment (heating at 353 K) indicates that the particles of the partially and/or fully crystalline phase are nuclei (Figure 1A) for further crystallization of zeolite (Figure 1B and C) (Kosanović et al., 2008).

Lipidomics

The combination of studies in lipidomics with those of free radical modifications of lipids forms a basis for a chemical biology approach to the study of molecular mechanisms in a biological environment. The search for the correlations between our studies in free radical lipid peroxidations and lipid isomerizations forms the subject of the interdisciplinary collaboration among the European research groups within the COST Action "Free Radicals in Chemical Biology" (Chatgililoglu et al., 2008).



Figure 2. Particle size analyzer Mastersizer 2000.

Organic polymers

Initiation of crosslinking of unsaturated polyester (UPE) resins by ionizing radiation helped to identify the real cause of double peaks that often appear in crosslinking DSC thermograms of those resins and are usually assigned to initiator effects. We excluded the initiator by radiation initiation of the reaction and NMR spectroscopy detected the presence of ortho-phthalic saturated units in polyester of such resin. In the UPE-resin-containing iso-phthalic units, a single peak appeared in DSC thermograms. Presence of

ortho-phthalic units in polyester reduces its compatibility with styrene, probably because of steric hindrances what lead to a reaction-induced phase separation that increases homopolymerization, lowers the extent of crosslinking and causes the appearance of double peaks. Further literature reviewing revealed that double peaks in DSC thermograms almost exclusively appeared in ortho-phthalic-containing UPE resins while single peaks are characteristic of iso-phthalic-containing resins (Pucić et al., 2008).

Unusual oxidation of the intermetallic compound $Zr_{50}Cu_{50}$

The oxidation behaviour of selected zirconium based hydrogen-storage materials was investigated. Alloys of the composition $Zr_{50}Cu_{50}$ were prepared and their interaction with dry oxygen at high temperatures was studied (Paljević et al., 2008). A preferential oxidation of zirconium occurs within the temperature region 770 - 970 K, while the excess of copper is accumulated at the alloy-oxide interface forming the $Zr_{14}Cu_{51}$ phase. At 1100 K, after a strong exothermic reaction, the complete oxidation of the alloy into ZrO_2 and CuO occurs after 21 hours. The oxidation process showed an anomalous decrease of oxygen consumption in the temperature region 900 – 1000 K. This increase of oxidation resistivity was ascribed to preferentially oriented crystallites of ZrO_2 which have been formed within the oxide layer during oxidation. The reaction kinetics obeys a parabolic law with an activation energy of about 92 kJ/mol.

Supramolecular motifs and solvatomorphism within the compounds containing $[M(bpy)_3]^{2+}$ entities

Modern ideas in the design of new molecular solids with desirable physical properties are based on the analysis of controlled supramolecular aggregation of molecular entities. A specific type of supramolecular contact comprising four bipyridine ligands from two neigh-

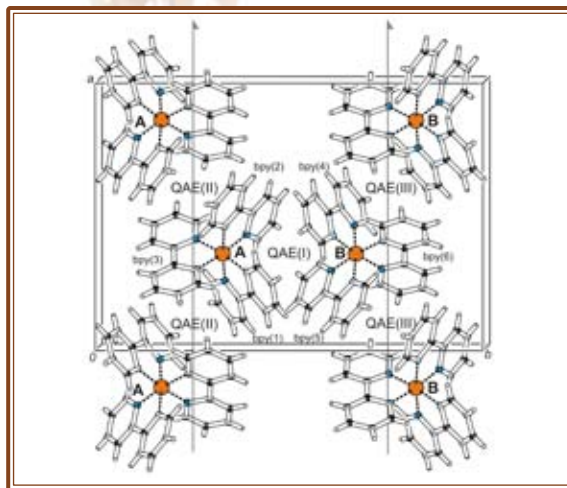


Figure 3. The QAE contacts comprising four bpy ligands from the two neighbouring $[M(bpy)_3]^{2+}$ cations in the orthorhombic crystal form of the new solvatomorphs.

bouring $[M(bpy)_3]^{2+}$ cations – quadruple aryl embrace (QAE) contact – has been revealed in the series of nine (9) new compounds of the composition $[M(bpy)_3]_2[NbO(C_2O_4)_3]Cl \cdot nH_2O$ ($M = Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}$ and Zn^{2+} ; $bpy = 2,2'$ -bipyridine), crystallizing in the monoclinic space group $P2_1/c$ ($n = 11$) or in the orthorhombic space group $P2_12_12_1$ ($n = 12$). The monoclinic form is a racemic structure containing an equal number of different $[M(bpy)_3]^{2+}$ enantiomers (δ and λ), whereas the orthorhombic form is an enantiopure structure containing only one type of $[M(bpy)_3]^{2+}$ enantiomers (δ or λ). Transformation of the monoclinic crystals into the more stable orthorhombic form during crystallization is a process of spontaneous resolution of the racemic compounds $[M(bpy)_3]_2[NbO(C_2O_4)_3]Cl \cdot 11H_2O$ ($M = Fe^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+}$) into the racemic conglomerates $[M(bpy)_3]_2[NbO(C_2O_4)_3]Cl \cdot 12H_2O$. The two structural forms differ in composition just in the number of solvate (water) molecules (11 versus 12); therefore, this series of compounds exhibits the phenomenon of solvatomorphism (Jurić et al., 2008).

Novel methods for assessing fish blood biochemical data

Using novel machine learning techniques, the authors created and generated compre-

hensible classification models for exploring the importance of blood chemistry parameters, strength, mutual interactions or dependencies, and reliability of particular parameters within the seasonal groups, for the first time (Čož-Rakovac et al., 2008).

NEW EQUIPMENT

A new dynamic laser light scattering particle size analyzer Mastersizer 2000 (Malvern) was obtained. The measurement range is 20 – 3000 nm of small quantity (50 – 100 mg) of solid sample dispersed in 1 – 2 ml of solvent (aqueous and/or organic). The instrument is used within a cooperative effort involving Ruđer Bošković Institute and Bartex-Bartol.

As part of a cooperative effort involving Ruđer Bošković Institute and Chiyoda Technol, we secured a radiophotoluminescent reader with dosimeters (FGD - 1000 for GD-300 series). A Varian capillary gas chromatograph GC 450 equipped with a flame ionization detector was obtained.

In addition, the Division obtained an Electrophoresis set, a DNA imaging system and a PCR thermal cycler.

EDUCATION

Scientists from the Division contributed to 17 undergraduate and postgraduate courses in 2008 as part of the involvement in the educational programs of Universities in Zagreb, Osijek and Dubrovnik.

PATENTS

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

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Sciences, Education and Sports

1. Synthesis and microstructure of metal oxides and oxide glasses, Svetozar Musić
2. Polynuclear metal systems – synthesis and properties, Pavica Planinić
3. Metal hydrides in clean energy systems, Želimir Blažina
4. Study of influence of aluminosilicate precursors on their transformations, Boris Subotić
5. Precipitation mechanism of inorganic biocompatible and related materials, Damir Kralj
6. Structure-property relationships of modified polymer materials, Ivan Šmit
7. Physico-chemical effects of ionizing radiations in materials, Dušan Ražem
8. Subcellular biochemical and phylogenetic diversity of aquatic organisms, Rozelindra Čož-Rakovac

Programs supported by the Ministry of Sciences, Education and Sports

1. New functional materials, Svetozar Musić

Research, developmental and international projects

1. Metal oxides: structural and magnetic properties, Mira Ristić (Croatian-Serbian Scientific Cooperation Programme for 2008-2010).
2. Free Radicals in Chemical Biology (CHEM-BIORADICAL), Branka Mihaljević; Project number COST Action CM0603
3. Solid state dosimetry systems for various dosimetry fields, Maria Ranogajec-Komor; Bilateral scientific and technical co-operation between Croatian Academy of Sciences and Arts and Hungarian Academy of Science (2007 – 2009).
4. Characterization, intercomparison and application of radiophotoluminescence (RPL) dosimetry system according to international standards and protocols, Maria Ranogajec-Komor; Scientific co-operation between Ruđer Bošković Institute and Chiyoda Technol. Corporation, Japan; Signed 2 September 2008.

5. Nuclear techniques for the protection of the cultural heritage in the Mediterranean Region, Branka Katušin-Ražem; International Atomic Energy Agency Regional Technical Co-operation Project; Project number: RER/1/006
6. Quality control methods and procedures for radiation technology, Dušan Ražem; International Atomic Energy Agency Regional Technical Co-operation Project; Project number: RER/8/010
7. Optimization of the synthesis process of zeolite A with special emphasis on the control of particulate properties (size and shape of zeolite A crystals), Boris Subotić (Bartex-Bartol and Ruđer Bošković Institute co-operation scientific research – 2nd phase).
8. Atomic-force microscopy study of the crystallization of zeolites A, X and silicalite from amorphous (alumino)silicates, Cleo Kosanović (Croatian-Hungarian Intergovernmental Science and Technology Cooperation Programme for 2007-2009).
9. PHARE project: "Trout and Tourists", Rozelindra Čož-Rakovac (Department for Financing EU Assistance Programmes and Projects, Central Finance and Contracting Unit, 2005-0808-010101)
10. VIP project: "Model of revitalization and breeding of brown trout", Rozelindra Čož-Rakovac (Ministry of Agriculture, Forestry and Water Management MAFWM, VI-1-10/05)
11. VIP project: "Preservation of oyster production by asserting its autochthony" Ivančica Strunjak-Perović (Ministry of Agriculture, Fisheries and Rural Development, VIII-5-50/08)
12. "Determination of genetic structure and restoration of autochthonous population of brown trout in the National Park Plitvice Lakes", Rozelindra Čož-Rakovac (National Park Plitvice Lakes/Ministry of Environmental Protection, Physical Planning and Construction 21320/06)
13. Scientific/professional management of a project: "Breeding and Selection in Aquaculture", Fishery 1961 d.o.o., Mato Hacmanjek (MAFWM, 324-01/06-01/202)
14. Scientific/professional management of a project: "Breeding and Selection in Aquaculture", Fishery Vrnjika, Rozelindra Čož-Rakovac (MAFWM, 324-01/06-01/215)
15. Scientific/professional management of a project: "Breeding and Selection in Aquaculture", Gacka d.o.o., Natalija Topić Popović (Ministry of Agriculture, Fisheries and Rural Development 324-01/08-01/393)
16. Scientific/professional management of a project: "Breeding and Selection in Aquaculture", Fishery 1961 d.o.o., Ivančica Strunjak-Perović (Ministry of Agriculture, Fisheries and Rural Development 324-01/08-01/401)
17. Aquatic animal health monitoring – contracts with 8 international and national companies, Rozelindra Čož-Rakovac, Mato Hacmanjek

INVITED LECTURES

1. Topić Popović, N. Good laboratory practice in manipulation with fish as a model in biomedical research. 5th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 27, 2008.
2. Jadan, M. Genetic structure of brown trout population, 5th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 27, 2008.
3. Strunjak-Perović, I. Diseases of crayfish, 5th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 27, 2008.
4. Čož-Rakovac, R. Crayfish Farming. 5th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 27, 2008.
5. Ranogajec-Komor, M. Application of solid state dosimeters in individual, medical and environmental dosimetry. Sapientia University, Cluj, Romania, 1 April 2008.
6. Ranogajec-Komor, M. Environmental monitoring with solid state dosimeters. Advanced Training Course "New Techniques for the Detection of Nuclear and Radioactive Agents", Mugla, Turkey, 26 – 30 May 2008.
7. Ražem, D. Effects of radiation on controlled drug delivery and release systems. 15th International Meeting on Radiation Processing. Workshop on Radiation Sterilization of Drug – Device Combination Products. London, United Kingdom, 21 – 25 September 2008.
8. Miljanić, S. Double dosimetry in interventional radiology – practice, evaluation and recommendations. 4th International Workshop on Individual Monitoring, Oarai, Japan, 1-3 December, 2009.

ORGANIZED CONFERENCES

XXIX. European Congress on Molecular Spectroscopy (EUCMOS-2008), Opatija, 31.08.-05.09.2008., Chairpersons: Svetozar Musić and Krešimir Furić (Ruđer Bošković Institute).

The First Croatian Symposium on Zeolites, Split (Croatia) 26-27.09.2008. Organization: Croatian Zeolite Association, Ruđer Bošković Institute and University of Split. President of the Organizing Committee: Josip Bronić (Ruđer Bošković Institute).

SELECTED PUBLICATIONS

1. Gotić M, Musić S. Synthesis of nanocrystalline iron oxide particles in the iron(III)acetate/alcohol/acetic acid system. *Eur J Inorg Chem* 2008: 966.
2. Kontrec J, Kralj D, Brečević Lj, Falini G. Influence of some polysaccharides on the production of calcium carbonate filler particles. *J Cryst Growth* 2008: 310: 4554.
3. Kosanović C, Bosnar S, Subotić B, Svetličić V, Mišić T, Dražić G, Havenscak K. Study of the microstructure of amorphous aluminosilicate gel before and after its hydrothermal treatment. *Micropor Mesopor Mat* 2008: 2-3: 177.
4. Chatgililoglu C, Ferreri C, Hermetter A, Lacote E, Mihaljević B, Nicolaides A, Siafaka-Kapadai A. Lipidomics and free radical modification of lipids. *Chimia (Basel)* 2008: 62: 713.
5. Pucić I, Jurkin T. Radiation and Postirradiation Crosslinking and Structure of Two Unsaturated Polyester Resins. *Polym Engin Sci* 2008: 48: 1768.

6. Paljević M, Tudja M. Unusual oxidation behaviour of $Zr_{50}Cu_{50}$ alloy at high temperatures. *Corros Sci* 2008: 50: 818.
7. Jurić M, Perić B, Brničević N, Planinić P, Pajić D, Zadro K, Giester G, Kaitner B. Supramolecular motifs and solvatomorphism within the compounds $[M(bpy)_3]_2[NbO(C_2O_4)_3] \cdot nH_2O$ ($M = Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}$ and Zn^{2+} ; $n = 11, 12$). Syntheses, structures and magnetic properties. *Dalton Trans* 2008: 742.
8. Čož-Rakovac R, Šmuc T, Topić Popović N, Strunjak-Perović I, Hacmanjek M, Jadan M. Novel methods for assessing fish blood biochemical data. *J Appl Ichthyol* 2008: 24: 77.

Chapters in Books

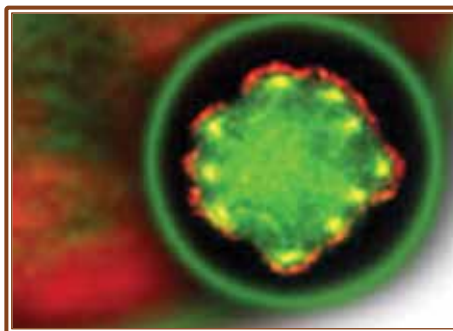
1. Subotić B, Bronić J, Antonić Jelić T. Theoretical and Practical Aspects of Zeolite Nucleation. In: *Ordered Porous Solids: Recent, Advances and Prospects*. Editors: Mintova, Svetlana; Valtchev, Valentin; Tsapatsis, Michael. Elsevier, Amsterdam, 2008, pp 127-185.
2. Ražem D. Radiation sterilization of pharmaceuticals: An overview of the literature. In: *Trends in Radiation Sterilization of Health Care Products*. International Atomic Energy Agency, Vienna, 2008, pp 175-185.
3. Chu RDH, Desrosiers MF, Inokuti M, Klassen NV, Kovacs A, McLaughlin WL, Miller A, Ražem D, Sharpe PHG, Shortt K, Seltzer SM, Takehisa M, Tanaka R, Whittaker B, Wieser A. Dosimetry systems. In: *Dosimetry Systems for Use in Radiation Processing*. International Commission on Radiation Units and Measurements (ICRU) Report No. 80. ICRU, Bethesda, MD, 2008, pp. 29-70.

DIVISIONAL ORGANISATION

Head: Igor Weber

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

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



Model organisms used in these studies include bacteria, yeast and other fungi, cellular slime moulds, several invertebrates, plants and mammalian cells. The projects in our Division broadly comprise the following fields of study: maintenance of genome integrity and regulation of genome variation (DNA replication, recombination and repair); genome organization and repetitive DNA sequences; expression of genomic information (transcription and translation); signal transduction in molecular regulation of cell division, growth, differentiation and senescence; cellular responses to toxic agents and resistance to cytostatics and antibiotics; genetic background and regulatory mechanisms of neurotransmission; regulatory mechanisms of photosynthesis; physiology, biochemistry and structural biology of plant hormones; antioxidant activity of polyphenols; fungal biodiversity including taxonomy, biogeography and ecology of fungi; dynamical processes in the cytoskeleton; and evolution of genes and genomes. The primary purpose of these research projects is a general broadening of our knowledge of biological processes at the molecular level and the underlying principles of life, as well as the training of young scientists for professional work in the field of molecular biosciences, including biomedicine and biotechnology.

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.

In 2008, members of the Division of molecular biology participated in the teaching of more than 30 undergraduate and postgraduate courses at Croatian universities. During that year they also supervised more than 20 diploma, M.Sc., and Ph.D. theses. A series of practical courses in biology and medicine was organized in our Division by Andreja Ambriović Ristov (<http://www.tecajevi-irb.com>).

TOP ACHIEVEMENTS

Gene expression and transcriptional regulation in lymphoma

We analyzed gene expression and transcriptional regulation in lymphocytes from patients with lymphoma compared to normal lymphocytes. We tackled the question whether there is a quantitative difference in distribution of Ikaros, Aiolos, and Helios mRNA between Hodgkin lymphoma (HL) and non-Hodgkin lymphoma (NHL). Formalin-fixed and paraffin embedded sections of lymph nodes from patients were analyzed by real time qRT-PCR. Ikaros and early B-cell factor (EBF) transcription factors regulate lambda 5 expression of pre-B-cell receptor (BCR) at the pre-BI stage of B-cell development. The transition from pre-BI to pre-BII is marked by pre-BCR down-regulation due to higher Aiolos expression. Because one approach to understanding neoplastic transformation is by comparing normal cells to their

malignant counterparts, our results would indicate a dysregulation of a developmental pathway in follicular centre cell lymphoma (FCC-NHL). Our results show for the first time Aiolos overexpression in primary lymphoma tissues (Antica et al., 2008).

Transcription of centromeric DNA

Non-coding RNA deriving from centromeric regions is proposed to play an active role in the formation of pericentromeric and centromeric heterochromatin, both of them important for proper centromere function. We have identified and characterized stable, RNA polymerase II dependant transcripts of abundant centromeric satellite DNA, not regulated by RNAi, in beetle *Tribolium castaneum* (Pezer and Ugarković, 2008a). The functional studies indicate that slight changes in expression of non-coding centromeric RNA could induce chromosome instability, mis-segregation and aneuploidy, facilitating

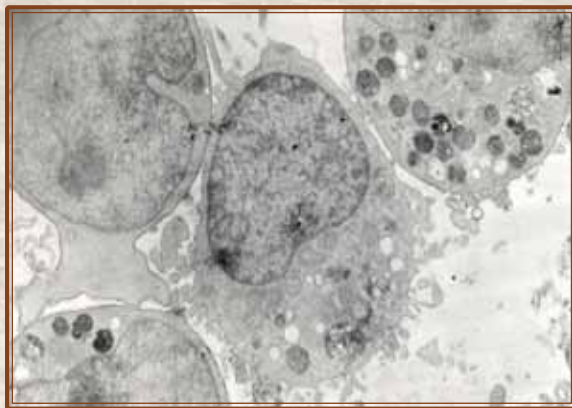


Figure 1. Mitogen-stimulated lymphocytes, TEM.

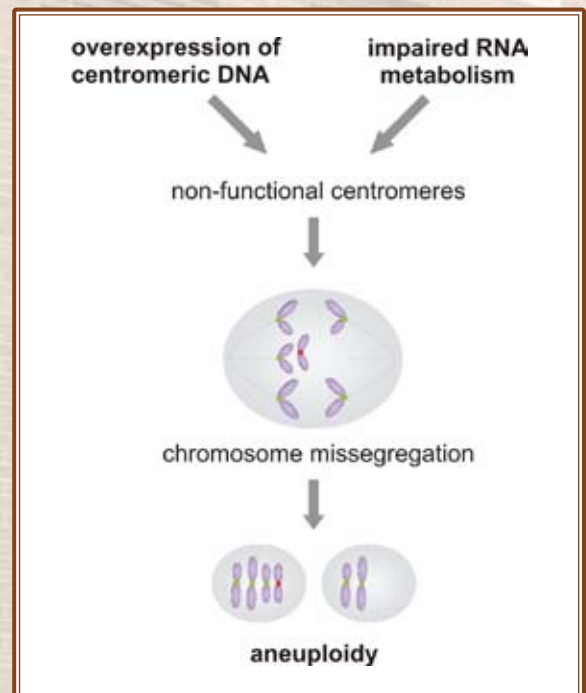


Figure 2. Link between centromeric RNA and aneuploidy. Aberrant expression of centromeric satellite DNA affects centromere/kinetochore function and causes abnormality in chromosome segregation. Defects in RNA metabolism could affect heterochromatin maintenance and fidelity in mitosis.

finally tumourigenesis (reviewed in Pezer and Ugarković, 2008b).

Integrin-mediated drug resistance

Recently, we found the up-regulation of $\alpha\beta 3$ integrin in human laryngeal carcinoma cells resistant to cisplatin. We show here, on the model of human laryngeal carcinoma-derived $\alpha\beta 3$ integrin-expressing cells, the appearance of resistance to several anti-cancer drugs (cisplatin, mytomyacin C and doxorubicin). Our results describe a novel mechanism mediated by $\alpha\beta 3$ integrin that is the consequence of glutathione-dependent increased ability of $\alpha\beta 3$ integrin-expressing cells to eliminate drug-induced reactive oxidative species (Brozović et al., 2008).

An ancient evolutionary origin of human disease genes



Figure 3. An artistic illustration of phylostratigraphy.

Genomic phylostratigraphy of human genetic diseases shows that evolutionary origin of disease genes is not random. Surprisingly, there is a clear bias towards old genes, whereas disease genes specific to the mammalian lineage are almost absent. These regularities show that genetic diseases are an inescapable component of life and that all living organisms today, i.e. not only humans, will be affected by similar genetic diseases. The article was evaluated in "Faculty of 1000 Biology" and reports about it were published in "New Scientist" and "The Economist" (Domazet-Lošo and Tautz, 2008).

MODERN FACILITIES, METHODS AND EQUIPMENT

Centre for DNA sequencing

The DNA centre for DNA sequencing, under the supervision of Helena Četković as part of the Laboratory for Molecular Genetics, continued to provide services during 2008. Besides DNA sequence analyses, it also offers a microsatellite genotyping method for external users. More than 2500 sequence analyses were performed in this year at the DNA centre using ABI-Prism 3100 Sequencer.

Confocal laser scanning microscope

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

GBOX EF Gel Documentation System

A new, cost-effective gel documentation system from Syngene is capable of accurately producing images of gels and blots stained with both visible and low-light emitting fluorescent dyes.



Figure 4. The new gel documentation system.

AWARDS

Ruđer Bošković Institute, as the publisher, was awarded the “Josip Juraj Strossmayer Award” by the Croatian Academy of Science and Arts for the best publication in Croatian language in natural sciences in 2007 for the book “Metode u molekularnoj biologiji” (Methods in molecular biology, Editor in chief: Andreja Ambriović Ristov).

Scientific Excellence Award granted by Croatian Ministry of Sciences, Education and Sports, for the article: Piljac-Žegarac J, Valek L, Martinez S, Belščak A. Fluctuations in the phenolic content and antioxidant capacity of dark fruit juices in refrigerated storage. Food Chem 2008 (<http://dx.doi.org/10.1016/j.foodchem.2008.07.048>). This journal is ranked 4th of 103 in the category “Food science and technology” according to the Journal Citation Report (Jasenka Piljac Žegarac).

EDUCATION

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

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Sciences, Education and Sports

1. Increase of adenovirus transduction efficacy and resistance to cytostatics, Andreja Ambriović Ristov
2. Serotonergic transmission: genes, proteins and behavior, Branimir Jernej
3. Molecular regulation of plant development, Branka Salopek-Sondi
4. Hydrodynamics of cerebrospinal fluid, Darko Orešković
5. Molecular mechanisms of DNA recombination and repair, Davor Zahradka
6. Fundamental molecular studies of Streptomyces biology, Dušica Vujaklija

7. Evolution and function of fast evolving portion of eukaryotic genome, Đurđica Ugarković
8. Genes and genomes: structures, functions and evolutions, Helena Četković
9. Regulatory mechanisms of photosynthesis and differentiation of plastids, Hrvoje Fulgosi
10. Regulation of the cytoskeleton dynamics in cell motility and cytokinesis, Igor Weber
11. Molecular mechanisms of immortalization and cellular aging, Ivica Rubelj
12. The role of recombination in DNA repair and genome evolution, Krunoslav Brčić-Kostić
13. Serotonergic mechanisms in alcoholism, Lipa Čičin-Šain
14. Cell response to cytotoxic agents and resistance development, Maja Osmak
15. Molecular interactions in lymphocyte differentiation, Mariastefania Antica
16. Transcriptional regulation in eukaryotes, Mary Sopta
17. Evolution, properties and functional interactions of satellite DNA sequences, Miroslav Plohl

Program supported by the Ministry of Sciences, Education and Sports

1. Molecular fundamentals of biological processes, Miroslav Plohl.

Research, developmental and international projects

1. Structural and functional analysis of noncoding heterochromatic DNA in insect *Tribolium castaneum*, Đurđica Ugarković (EC FP6 Marie Curie Transfer of Knowledge project MTKD-CT-2006-042248)
2. Exploratory workshop on heterochromatin structure and function: from repetitive DNA sequences to epigenetics, Miroslav Plohl (European Science Foundation grant, ESF-EW 07-032)
3. Biophotonics approach to regulation of the actin cytoskeleton dynamics by small GTPase proteins, Igor Weber (UKF 1A Grant Agreement 9/07)
4. Transcriptional regulation in human leukemic cells, Mariastefania Antica (MSES, bilateral project with Austria, 910-08/07-01/00129)
5. Subcellular localization of glutathione and cysteine in cyanobacteria, Hrvoje Fulgosi

- (MSES, bilateral project with Austria, 910-08/07-01/00125)
6. Study of DNA, protein components and their interactions in holocentric chromosomes of root-knot nematodes of the genus *Meloidogyne*, Miroslav Plohl (MSES, Cogito bilateral project with France, 910-08/06-01/00093)
 7. Adenovirus retargeting to aminopeptidase N and potential application in gene therapy of cystic fibrosis, Andreja Ambriović Ristov (MSES, Cogito bilateral project with France, 910-08/06-01/00098)
 8. Analysis of cytoskeleton dynamics during phagocytosis and cell migration, Igor Weber (MSES, DAAD bilateral project with Germany, 910-08/07-01/00143)
 9. Molecular mechanisms determining cellular susceptibility to platinum drugs, Maja Osmak (MSES, DAAD bilateral project with Germany, 910-08/07-01/00145)
 10. Plant hormones in development and biotic stress using biochemical and molecular approaches, Branka Salopek-Sondi (MSES, bilateral project with Slovenia, 919-08/06-01/00208)
 11. Bacterial endophytes, a novel biosource for biocatalytic, agricultural and environmental application, Dušica Vujaklija (FWF - Translational Research Program, No: L129)
 12. Certified laboratory for the analysis of antioxidants in food products, Jasenka Piljac Žegarac (HITRA-TEST, E38-2005)
 13. Regeneration of articular cartilage of the knee, Andreja Ambriović Ristov (MSES, HITRA-TEST, 381-01/06-02/00032)
 14. Propagation of the American highbush blueberry (*Vaccinium corymbosum* L.), Branka Salopek-Sondi (Centre for agriculture at high altitudes, Primorsko-goranska county, applied collaborative project)
 15. Improving the quality of products based on sour cherry maraska juice, Helena Četković (Maraška Ltd., MPŠVG, 24-14/07)
- Symposium on Molecular Medicine. Heronissos, Greece, October 9-11, 2008.
2. Meštrović N, Plohl M, Castagnone-Sereno P: Relevance of satellite DNA genomic distribution in phylogenetic analysis: a case study with root-knot nematodes of the genus *Meloidogyne*. COST 872 - Exploiting genomics to understand plant-nematode interaction. Postojna, Slovenia, May 26-29, 2008.
 3. Vujaklija D: Tyrosine phosphorylation of bacterial SSBs from taxonomically distant bacterial species. Congress of the Slovenian Microbiological Society with International Participation. Portorož, Slovenia, November 19-22, 2008.
 4. Plohl M: Tandem repetitive DNA sequences in (peri)centromeric regions. ESF Exploratory Workshop on Heterochromatin structure and function: from repetitive DNA sequences to epigenetics. Donja Stubica, Croatia, September 20-23, 2008.
 5. Ambriović-Ristov A: General properties of adenoviruses: Virus structure and its molecular biology. FEMS course, Adenoviruses: from basic biology to gene therapy. Zadar, Croatia, September 23-24, 2008.
 6. Fulgosi H: Photosynthesis requires TROL. Scientific Symposium 50 Years of Molecular Biology in Croatia. Zagreb, Croatia, November 20-21, 2008.
 7. Mravinac B: Satellite DNAs in closely related species: the case of *Tribolium* beetles. ESF Exploratory Workshop on Heterochromatin structure and function: from repetitive DNA sequences to epigenetics. Donja Stubica, Croatia, September 20-23, 2008.
 8. Majhen D: Integrin $\alpha\beta3$: Link between resistance to cisplatin and adenovirus transduction efficacy. FEMS course, Adenoviruses: from basic biology to gene therapy. Zadar, Croatia, September 23-24, 2008.
 9. Meštrović N: Satellite DNAs in insect models – *Tribolium*. ESF Exploratory Workshop on Heterochromatin structure and function: from repetitive DNA sequences to epigenetics. Donja Stubica, Croatia, September 20-23, 2008.
 10. Zahradka K, Slade D, Bailone A, Sommer S, Averbek D, Petranović M. Lindner A, Radman M: DNA repair in radiation resistant bacterium *Deinococcus radiodurans*. HD-BMB2008 - Congress of the Croatian Society of Biochemistry and Molecular Biology with

SELECTED INVITED LECTURES

1. Osmak M, Brozović A, Čimbora-Zovko T, Majhen D, Fritz G, Ambriović Ristov A: Changes in cell adhesion proteins induced by the treatment with cisplatin and their role in cisplatin- resistance. 13th World Congress on Advances in Oncology and 101th International

- International Participation. Osijek, Croatia, September 17-20, 2008.
11. Piljac Žegarac J, Martinez S, Valek L, Stipčević T, Belščak A, Šamec D: Total phenol content and antioxidant capacity of Croatian food products – an overview. XII. Ružička days. Vukovar, Croatia, September 18-19, 2008.
 12. Meštrović N, Plohl M: Satellite DNAs: secret parts of genomes. Scientific Symposium 50 Years of Molecular Biology in Croatia. Zagreb, Croatia, November 20-21, 2008.
 13. Zahradka K: *Deinococcus radiodurans* – a radiation resistant bacterium. 7th Symposium of the Croatian Radiation Protection Association with International Participation. Opatija, Croatia, May 29-31, 2008.
 14. Harcet M, Četković H, Perina D, Müller W, Vlahoviček K: Comparative genomics reveals broad genetic repertoire of simplest metazoans – sponges (Porifera). Scientific Symposium 50 Years of Molecular Biology in Croatia. Zagreb, Croatia, November 20-21, 2008.
 15. Zahradka K, Buljubašić M, Petranović M, Zahradka D: Exol and SbcCD nucleases cooperate with RecBCD enzyme in reckless chromosome degradation in *recA* mutants of *Escherichia coli*. Fourth Croatian Congress of Microbiology with International Participation. Zadar, Croatia, September 24-27, 2008.

SELECTED ORGANIZED CONFERENCES

1. 50 Years of Molecular Biology in Croatia - Scientific Symposium. Zagreb, Croatia, November 20-21, 2008, Plohl M, Zahradka K.
2. ESF Exploratory Workshop on Heterochromatin structure and function: from repetitive DNA sequences to epigenetics. Donja Stubica, Croatia, September 20-23, 2008, Plohl M.
3. 4th Croatian Congress of Microbiology with International Participation. Zadar, Croatia, September 24-27, 2008, Vujaklija D.
4. FEMS course, Adenoviruses: from basic biology to gene therapy. Zadar, Croatia, September 23-24, 2008, Ambriović Ristov A.
5. Summer School Microbial Secondary Metabolites: Genomes, Signals and Communities. Dubrovnik, Croatia, August 24 - September 1, 2008, Vujaklija D.

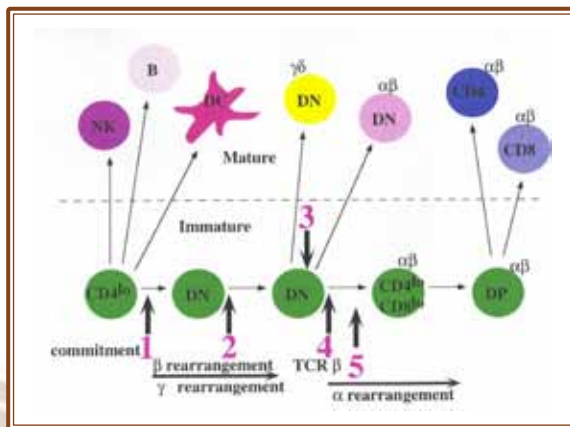


Figure 5. Development in the thymus from committed hematopoietic stem cell to immunocompetent cells.

SELECTED PUBLICATIONS

Research articles

1. Antica M, Čičin-Šain L, Kapitanović S, Matulić M, Džebro S, Dominis M. Aberrant Ikaros, Aiolos and Helios expression in Hodgkin and non-Hodgkin lymphoma. *Blood* 2008; 111: 3296.
2. Domazet-Lošo T, Tautz D. An ancient evolutionary origin of genes associated with human genetic diseases. *Mol Biol Evol* 2008; 25: 2699.
3. Castaldo G, Zucko J, Heidelberger S, Vujaklija D, Hranueli D, Cullum J, Wattana-Amorn P, Crump MP, Crosby J, Long PF. Proposed arrangement of proteins forming a bacterial type II polyketide synthase. *Chem Biol* 2008; 15:1156.
4. Brozović A, Majhen D, Roje V, Mikac N, Jakopec S, Fritz G, Osmak M, Ambriović-Ristov A. $\alpha\beta3$ integrin mediated drug resistance in human laryngeal carcinoma cells is caused by glutathione dependent elimination of drug induced reactive oxidative species. *Mol Pharmacol* 2008; 74: 298.
5. Sondi I, Škapin SD, Salopek-Sondi B. Biomimetic precipitation of nanostructured colloidal calcite particles by enzyme-catalyzed reaction in the presence of magnesium ions. *Cryst Growth Des* 2008; 8: 435.
6. Piljac-Žegarac J, Valek L, Martinez S, Belščak A. Fluctuations in the phenolic content and antioxidant capacity of dark fruit juices in refrigerated storage. *Food Chem* 2008 (Epub ahead of print: <http://dx.doi.org/10.1016/j.foodchem.2008.07.048>).

7. Salopek-Sondi B, Vukelić B, Špoljarić J, Šimaga Š, Vujaklija D, Makarević J, Jajčanin N, Abramić M. Functional tyrosine residue in the active center of human dipeptidyl peptidase III. *Biol Chem* 2008: 389: 163.
8. Pezer Ž, Ugarković Đ. RNA Pol II Promotes Transcription of Centromeric Satellite DNA in Beetles. *PLoS ONE* 2008a: 3: e1594.

Chapters in books

1. Ugarković Đ. Evolution of Alpha Satellite DNA. In: *Encyclopedia of Life Sciences (ELS)*, John Wiley & Sons, Ltd., Chichester 2008: <http://www.els.net>.

Invited review articles

1. Pezer Ž, Ugarković Đ. Role of non-coding RNA and heterochromatin in aneuploidy and cancer. *Semin Cancer Biol* 2008b: 18: 123.
2. Plohl M, Luchetti A, Meštrović N, Mantovani B: Satellite DNAs between selfishness and functionality: structure, genomics and evolution of tandem repeats in centromeric (hetero)chromatin. *Gene* 2008: 409: 72.
3. Vojta A, Fulgosi H, Schleiff E: The molecular concept of protein translocation across the outer membrane of chloroplasts. *Croat Chem Acta* 2008: 81: 511.



Division of Molecular Medicine

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

DIVISIONAL ORGANIZATION

Head: Krešimir Pavelić

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

- ⇒ Laboratory for Systems Biomedicine, Krešimir Pavelić
- ⇒ Laboratory of Experimental Hematology, Immunology and Oncology, Jelka Gabrilovac
- ⇒ Laboratory of Epigenomics, Koraljka Gall-Trošelj
- ⇒ Laboratory of Molecular Virology and Bacteriology, Magdalena Grce
- ⇒ Laboratory of Molecular Endocrinology and Transplantation, Mirko Hadžija
- ⇒ Laboratory of Functional Genomics, Marijeta Kralj
- ⇒ Laboratory for reactive radicals, Tatjana Marotti
- ⇒ Laboratory of Molecular Neuropsychiatry, Dorotea Muck-Šeler
- ⇒ Laboratory of Molecular Oncology, Jasminka Pavelić
- ⇒ Laboratory of Molecular Neuropharmacology, Danka Peričić
- ⇒ Group for Translational Medicine, Oliver Vugrek
- ⇒ Laboratory for Oxidative Stress, Neven Žarković
- ⇒ Laboratory for hereditary cancer, Sonja Levanat
- ⇒ Laboratory for personalized medicine, Sanja Kapitanović



OVERVIEW OF THE DIVISION

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

The Division is currently developing several strategic projects. These include the development of molecular targeted therapy for use against cancer and viral diseases, new diagnostic tools and research aimed at deciphering the molecular basis of disease, and tools based on -omics approaches. As such, the Division is emerging as a centre of excellence, for research in molecular approaches to the study of disease.

TOP ACHIEVEMENTS IN BASIC AND APPLIED RESEARCH

Curcumin's molecular mechanism of action in the context of epigenomic modulation

In the research on the mechanism of expression regulation of IGF2 and H19, H19 silencing in tumour cells upon curcumin treatment was induced, and the IGF2/H19 imprinting, CTCF and IGF2-R loss of heterozygosity and presence of H. Pilory in laryngeal squamous carcinomas in humans was analyzed (Novak Kujundić et al., 2007).

Mechanism of anticancer activity of novel quinoline derivatives

Using a proteomic approach based on 2DE coupled with a mass spectrometric mechanistic study, the N-amidino-substituted benzimidazo-1,2- α -quinoline was obtained. The quinoline derivative triggered transient, p53-independent G₂-M arrest in mutant p53 human colon cancer cells and succeeding mitotic transition, whereby these cells underwent cell death probably due to mitotic catastrophe. The antiproliferative effect of the quinoline derivative supports its possible role as an antimetastatic agent in colorectal carcinoma (Sedić et al., 2008).

Cooperation of antioxidative enzyme network

In ageing mouse liver and brain, stronger correlative links of antioxidative enzyme networks exist in old female mice than in old male mice demonstrating one possible reason why old females are better protected from oxidative stress than males (Sobočanec et al., 2008).

Granulocytes in spontaneous **regression of Walker 256 carcinoma**

Granulocytes were found to be effective host defence in the early stage of cancer. This finding explained for the first time the

well known phenomenon of spontaneous regression of Walker 256 carcinoma in rats (Jaganjac et al., 2008).

Lipidomics and lipid peroxidation using the yeast cell model

The cellular adaptation to metabolic changes induced by the synthesis of polyunsaturated fatty acids is associated with increased resistance to oxidative stress (Čipak et al., 2008).

Novel potential anticancer compounds

Over 150 newly synthesized compounds, such as urea and carbamate derivatives of primaquines, novel ketoprofen amides, fluoroalkylated pyrimidine derivatives, enediynes, glucosylated and adamantylated enkephalin analogues, adamantane substituted crown compounds and many others were screened *in vitro* for potential antitumor activity and the possible mechanisms of action were ascertained for the most effective ones (Kralj et al., 2008; Hranjec et al., 2008).

Antitumor therapy and **p21^{WAF1/CIP1}** gene

The molecular mechanisms underlying cell cycle and cell death were studied using cDNA-arrays and qPCR. The *p21* can assume a dual role in apoptosis in the same cell system depending on the chemotherapeutic agent: its over-expression enhances apoptosis in cisplatin-treated cells and attenuates apoptotic signals in methotrexate-treated cells. The observed dual role of *p21* was in direct correlation with the modulation of caspase 3 and 7 activation and changes in the expression of *GADD45a* gene (Kraljević Pavelić et al., 2008)

The influence of IL-8 and IL-10 on sporadic colon cancer development and progression

IL-10 SNP promoter genotypes were associated with increased risk of sporadic colon cancer. A significant increase in IL-8 and a decrease in IL-10 mRNA expression in tumour tissue compared with normal mucous tissue were observed. Positive IL-10 immunohistochemical reaction was more frequent in well differentiated tumours and IL-8 staining was more frequent in poorly differentiated tumours. These results indicate a possible tumour promoting role of IL-8 and tumour protective role of IL-10 in sporadic colon cancer (Čačev et al., 2008).

A novel therapeutic indication in bipolar depression

Six weeks of treatment with low doses of the antiepileptic drug lamotrigine significantly reduced depressed symptoms, and decreased platelet serotonin concentration in patients with bipolar depression, indicating that lamotrigine possesses an *in vivo* serotonin-uptake inhibiting property, and this effect might have contributed to its antidepressant activity (Šagud et al., 2008).

Patents

Kraljević Pavelić S, Cindrić M, Sedić M, Hock K, Pavelić K. Proteomic profile and protein detection methods in blood. P2008056A

MODERN FACILITIES, METHODS AND EQUIPMENT

The new Laboratory for systems biomedicine, which includes the Centre for Proteomics and Mass Spectrometry as well as the Centre for Transcriptomics, has been established. The Centre for Proteomics and Mass Spectrometry offers commercial services which include amino-acid, protein and peptide sequencing upon isolation and pu-



Figure 1. The 4800 Plus MALDI TOF/TOF[™] analyser that relies on the Matrix-assisted laser desorption/ionization MS.

rification. Additionally, the molecular weight analysis could be performed according to the MS and MS/MS measurements. Peptide and protein identification from complex mixtures is performed by using specialized software packages that are directly connected with publicly open databases such as The Protein Data Bank or SwissProt (Figure 1).

NEW METHODS

Breast cancer genes BRCA 1 and 2

The first screening for the breast cancer genes BRCA 1 and 2 was done in Croatia, with new sequence variants in BRCA1 and BRCA2 genes detected by high-resolution melting analysis in an elderly healthy female population.

Analysis of gene expression within intact mouse embryos

RNA whole mount *in situ* hybridization is a recently introduced method which enables analysis of gene expression within intact mouse embryos (Korolija M, Ph.D. thesis). Transcripts of target genes are hybridized with digoxigenin-labelled riboprobes and visualized *in situ* by an alkaline phosphatase detection system (Figure 2).

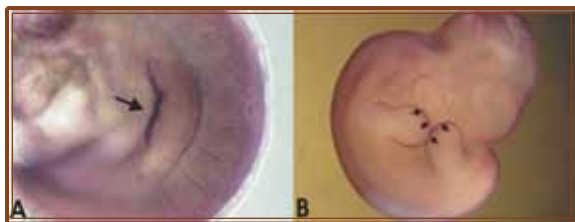


Figure 2. *Fgf 8* expression in the apical ectodermal ridge (AER, indicated by arrows) of the developing limb buds of mouse embryos at embryonic day 9.5 (a) and embryonic day 11.5 (b).

Genotyping assays for Human papillomavirus (HPV) types

Although there are more than 100 Human papillomavirus (HPV) types, only the high-risk (oncogenic) types cause cervical precancer and cancer (Figure 3). Due to the large number of HPV types, 4 genotyping assays were evaluated on a wide spectrum of less prevalent HPV types indicating that the use of only one assay in epidemiological and clinical studies might lead to biased conclusions (Sabol et al., 2008). In addition, a novel HPV type 16 variant with 63-nucleotides duplication in the E1 region was found. This particular variant found in 11% cervical specimens of 429 HPV 16 positive Croatian women show reduced oncogenicity, which is particularly interesting for the prediction of disease progression.

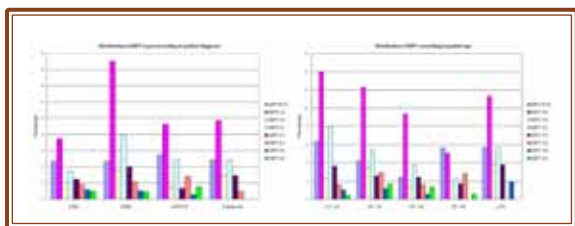


Figure 3. Distribution of Human Papilloma Virus (HPV) types in Croatia.

INTERNATIONAL FUNCTIONS

Krešimir Pavelić was appointed in November as a Secretary General of the European Molecular Biology Conference (EMBC) and *ex officio* member of the EMBO Council. Until November he was vice-president of the EMBC. Krešimir Pavelić is also member of the EMBC Strategic Working Party, Member

of the Standing Committee, European Medical Research Council, ESF. Krešimir Pavelić was appointed as a coordinator of the EU expert group for Stem cell therapy and regenerative medicine in European Medical Research Council, European Science Foundation (ESF). On the meeting of European Medical Research Council in The Royal College of Physicians in UK, Krešimir Pavelić initiated the revitalization of the project EuroSTELLS. Krešimir Pavelić is Editor of the Journal of Oncology and Central European Journal of Biology.

Nela Pivac was appointed as a member of the Regional CINP (Congress Internationale Neuro-Psychopharmacologicum) Committee for Southern and Eastern Europe.

Sonja Levanat was appointed as a Council member of European Association for Cancer Research (EACR).

Magdalena Grce was appointed as a delegate from RBI and a member of the Board of Directors of the European Cervical Cancer Association (ECCA).

DOMESTIC FUNCTIONS

Krešimir Pavelić is president of the National Scientific Council, president of the Governing Board of the Institute for Medical Research, Member of the Governing Board, Agency for Science and High Education, Ministry of Sciences, Education and Sports, and Dean in Department of Biotechnology at the University of Rijeka.

Tatjana Marotti was re-appointed as a member of the Board of Governors of Ruđer Bošković Institute.

AWARDS

FameLab 2008 award to Marko Košiček

Marko Košiček (Figure 4) received both the Croatian and International FameLab 2008 awards organized by the Festival of Science and the British council for the best scientific presentation. FameLab, originally

a UK talent competition, was established in 2005 and aims to find the best new talents in science communication.

Annual award for young researchers in biomedicine

Ana Šarić received the Annual award for young researchers in biomedicine from the Society of University Teachers, Scholars and Other Scientists – Zagreb for the year 2007. She was awarded for the excellent paper: Šarić et al., published in Neuroscience.

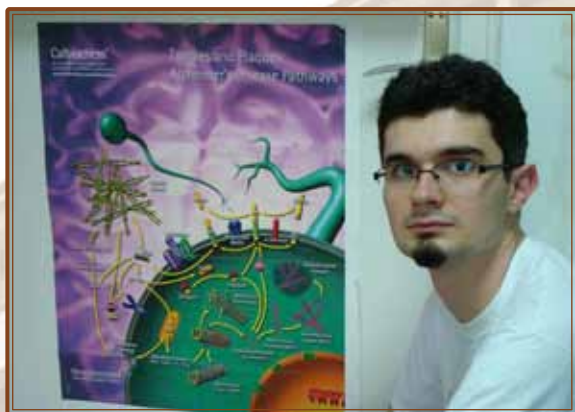


Figure 4. Marko Košiček

Award of the Croatian Academy of Science and Arts and The Zagreb Fair

Award of the Croatian Academy of Science and Arts and The Zagreb Fair to Institute Ruđer Bošković, the editor-in-chief Andreja Ambrović Ristov, and editors Anamaria Brozović, Branka Bruvo Mađarić, Helena Četković, Maja Herak Bosnar, Dubravka Hranilović, Silva Katušić Hećimović, Nevenka Meštrović Radan; Snježana Mihaljević, Neda Slade and Dušica Vujaklija for the best publishing achievement: Methods in Molecular Biology.

Spin Off Company

The spin off company, Ruđer-Medikol Diagnostics Ltd. (Figure 5), was established by Rudjer Innovations as its daughter com-

pany. This Company has started the hereditary breast cancer genetic testing, using a sophisticated method developed in the Division of Molecular Medicine at Rudjer Boskovic Institute, led by Sonja Levanat and her group. Genetic testing can reveal if person has a gene mutation associated with possible breast and ovarian cancer development. This testing analyzes BRCA1 and BRCA2 genes, which are often mutated in hereditary breast and ovarian cancer.



Figure 5. Rudjer-Medikol Diagnostics Ltd.

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sports

1. Molecular characteristics of the myo-fibroblasts in the Dupuytren's disease, Krešimir Pavelić
2. Role of membrane peptidases on tumour and normal cells, Jelka Gabrilovac
3. Epigenetic and Immunomodulatory Changes in Malignant Head and Neck Tumours, Korljka Gall Trošelj
4. Aberrant DNA methylation in HPV associated lesions, Magdalena Grce
5. Obtaining the structures like Langerhans islets from mouse stem cells, Mirko Hadžija
6. The role of nm23 genes in oral squamous cell carcinoma, Maja Herak Bosnar
7. Molecular genetics and pharmacogenetics of gastrointestinal tumours, Sanja Kapitanović
8. The mechanism(s) of cholesterol action in Alzheimer's disease, Silva Katušić Hećimović
9. The role of different cell death responses to DNA-damage treatment, Marijeta Kralj
10. Signal transduction in tumours: Hh-Gli interactions and therapeutic potential, Sonja Levanat

11. Cytochrome P450 monooxygenase and tumour appearance in ageing and oxidative stress, Tatjana Marotti
12. Immunopathogenesis of human recurrent herpes simplex virus infection, Zorica Mikloška
13. Pharmacogenomics and proteomics of serotonergic and catecholaminergic system, Dorotea Muck-Šeler
14. Gene therapy of tumours by modulating the molecules of immune system, Jasminka Pavelić
15. Stress, GABA-A receptors and mechanisms of action of neuropsychopharmacological drugs, Danka Peričić
16. Molecular basis and treatment of psychiatric and stress related disorders, Nela Pivac
17. New approaches in the treatment of malignant diseases, Marko Radačić
18. The role of p53/p73 protein network in soft tissue sarcoma, Neda Slade
19. Molecular characterisation of S-adenosylhomocysteine deficiency in humans, Oliver Vugrek
20. Lipids, free radicals and their second messengers in integrative oncology, Neven Žarković
6. Cellular sites of dual γ -secretase cleavage (Silva Katušić Hećimović, Bilateral project with Germany, co-investigators: Harald Steiner, Sven Lammich)
7. Hereditary Breast Cancer predisposition in Croatia and Hungary', (Croatian Hungarian Intergovernmental S&T Cooperation Programme 2007-2008, Sonja Levanat, Croatia, Edith Olah, Hungary)
8. Integrating and Strengthening Genomic Research in South East Europe (INTEGERS) FP7-REGPOT-2007-1 (Fran Borovečki, members of Coordination Committee: Dorotea Muck-Šeler, Nela Pivac)
9. Frontotemporal dementias and motor neuron disease (Rajka Liščić, Bilateral Cooperation with Slovenia; co-investigators: Dorotea Muck-Šeler, Nela Pivac)
10. Genetic testing of monogenetic diseases: cystic fibrosis, non-syndromic deafness, Rett syndrome, (Clinical Hospital Split, Children's Hospital Zagreb, Jasminka Pavelić)
11. Genetic factors as markers of suicide (Nela Pivac, Bilateral Cooperation with Slovenia; co-investigator: Dorotea Muck-Šeler)
12. The role of p73 in cell cycle control (Bilateral collaboration with France, Cogito, Neda Slade)
13. Development of vaccine against herpes genitalis (Croatian Fund for development and employment, Zorka Mikloška)
14. COST (European Cooperation in the field of Scientific and Technical Research) Action B35 "Lipid Peroxidation Associated Disorders" in the Domain Biomedicine and Molecular Biosciences, Action Chair Neven Žarković
15. Effects of the lipid peroxidation product 4-hydroxynonenal on primary hepatocytes, (Croatian-Austrian Science Technology Cooperation Program, Neven Žarković)
16. Support of human bone growth in vitro by bioactive glass and 4-hydroxynonenal, (Austrian National Bank Jubileums Fond Research Grant, Renate Wildburger (LKH Graz) and Neven Žarković)
17. Novel, genuine assays for lipid peroxidation analyses in experimental oncology, (Bilateral project on scientific and technological research collaboration with France – COGITO, Neven Žarković)
18. Modifying drug resistance by oxidative stress and antioxidants (Bilateral Hungarian – Croatian Scientific and Technological Collaboration project, Neven Žarković)

Programs supported by the Ministry of Science, Education and Sports

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

Research, developmental and international projects

1. Development of drugs for treatment of Dupuytren disease, (Croatian Fund for development and employment. Krešimir Pavelić).
2. Toxicological *in vivo* studies of Lectranal (MILSING Corp, Mirko Hadžija)
3. Therapeutic effects of mushroom extracts, (HITRA, Mislav Jurin)
4. The role of cholesterol in Alzheimer's disease (Alison Goate, NIH - Fogarty International Research Collaboration Award, USA, co-investigator: Silva Katušić Hećimović)
5. The mechanism(s) of cholesterol action in Alzheimer's disease (Silva Katušić Hećimović, Bilateral project with USA, co-investigator: Alison Goate)
6. Cellular sites of dual γ -secretase cleavage (Silva Katušić Hećimović, Bilateral project with Germany, co-investigators: Harald Steiner, Sven Lammich)
7. Hereditary Breast Cancer predisposition in Croatia and Hungary', (Croatian Hungarian Intergovernmental S&T Cooperation Programme 2007-2008, Sonja Levanat, Croatia, Edith Olah, Hungary)
8. Integrating and Strengthening Genomic Research in South East Europe (INTEGERS) FP7-REGPOT-2007-1 (Fran Borovečki, members of Coordination Committee: Dorotea Muck-Šeler, Nela Pivac)
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10. Genetic testing of monogenetic diseases: cystic fibrosis, non-syndromic deafness, Rett syndrome, (Clinical Hospital Split, Children's Hospital Zagreb, Jasminka Pavelić)
11. Genetic factors as markers of suicide (Nela Pivac, Bilateral Cooperation with Slovenia; co-investigator: Dorotea Muck-Šeler)
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17. Novel, genuine assays for lipid peroxidation analyses in experimental oncology, (Bilateral project on scientific and technological research collaboration with France – COGITO, Neven Žarković)
18. Modifying drug resistance by oxidative stress and antioxidants (Bilateral Hungarian – Croatian Scientific and Technological Collaboration project, Neven Žarković)

SELECTED ORGANIZED CONFERENCES

1. Čretnik M. Organisation of International Summer School Hottest Topics in Protein Research, MedILS, Split, Croatia, July 19-26, 2008.
2. Čretnik M. Asistent on EMBO Course EMBO Course on Ubiquitin and SUMO, MedILS, Split, Croatia, September 12-19, 2008.
3. Pivac N, Muck-Šeler D. Third Croatian Congress on the Stress Related Disorders with international participation: therapy of the stress related disorders, Rabac, Croatia, June 5-7, 2008.
4. Pivac N. European Pharmacological Society (EPHAR) 2008, Manchester, United Kingdom, July 13-17, 2008.
5. Pivac N, Muck-Šeler D. Fourth Croatian Congress of Alzheimer's disease with international participation, Rovinj, Croatia, October 8-11, 2008.

SELECTED LECTURES

1. Balog T, Sobočanec S, Šverko V, Krolo M, Ročić B, Marotti M, Marotti T. The influence of season on oxidant-antioxidant status in trained and sedentary subjects. 4th International Conference on Health, Fitness & Active Living, Athens, Greece, May 8-11, 2008.
2. Grce M. Cervical Cancer Prevention in Croatia. HPV in Human Pathology, Prague, Check Republic, May 1-3, 2008.
3. Grce M. Cervical Cancer Screening in Europe: The Status Quo. 9th International Workshop of Lower Genital Tract Pathology - HPV-Related Disease in the Vaccine Era: Time to Retire? Viareggio, Italy, May 22-24, 2008.
4. Grce M. HPV DNA Testing for Cervical Cancer Screening. 7th International Symposium on Molecular Diagnostics, Graz, Austria, May 22-24, 2008.
5. Grce M. Cervical Cancer Screening Programme: Follow-up and Integrating the Services of other Healthcare Professionals. Consensus Congress on Cervical Cancer Prevention in Bulgaria and 14th National Conference of Gynaecological Oncology, Nessebar, Bulgaria, September 18-21, 2008.
6. Grdiša M. Specific drug delivery by TAT-technology. BIT Life Sciences' World Cancer

Congress-2008, Shanghai, China, June 12-17, 2008.

7. Grdiša M. Delivery of specific targeted drugs into the cells by TAT-technology. EHRlich II – 2nd World Conference on Magic Bullets, Nurnberg, Germany, October 3-5, 2008.
8. Kralj M: Adenoviruses for gene therapy of cancer. International Workshop organized by Croatian Microbiological Society Adenoviruses: Basic biology to gene therapy. Zadar, September, 23-24, 2008.
9. Kralj M: Adenoviruses-mediated p53 or *p21 waf1/cip1* gene transfer and its impact on cancer therapy. International Workshop organized by Croatian Microbiological Society Adenoviruses: Basic biology to gene therapy. Zadar, September, 23-24, 2008.
10. Levanat S: Evasive role of Hh-Gli pathway in cancer genetics (with an introduction on the state of cancer genetics research in Croatia). Yale School of Medicine, Department of Genetics Clinical Rounds, New Haven, CT, USA; June 16, 2008.
11. Levanat S: Molecular diagnostics of inherited breast cancers. 3rd Slovenian Congress of Clinical Chemistry with international participation and 18th International Symposium of Slovenian Association for Clinical Chemistry and Croatian Society of medical Biochemists. Ljubljana, Slovenia; November 13-15, 2008.
12. Levanat S: Role of genetics in early breast cancer detection. Croatian Academy for Science and Art (HAZU), September 25, 2008.
13. Mück-Šeler D, Nedić G, Pivac N, Babić A, Grubišić-Ilić M, Kozarić-Kovačić D: Serotonergic receptors type 2A in posttraumatic stress disorder. 3rd Croatian Symposium on Stress Related Disorders with International Participation. The Therapy of Stress Related Disorders, Rabac, Croatia, June 5-7, 2008.
14. Mück-Šeler D, Mustapić M, Mimica N, Pivac N, Presečki P, Folnegović-Šmalc V: Dopamine-beta-hydroxylase in Alzheimer's disease. 4th Croatian Congress on Alzheimer's Disease with International Participation, Rovinj, Croatia, October 8-11, 2008.
15. Pavelić J: Gene therapy. Who decides for a fetus? 4th South-East European Bioethical Forum, Rijeka-Opatija, Croatia, September 3-8, 2008.
16. Pivac N, Nedić G, Mustapić M, Muck-Šeler D, Grubišić-Ilić M, Kozarić-Kovačić D. Biological and genetic markers and suicidal behaviour

in posttraumatic stress disorder. 3rd Croatian Symposium on Stress Related Disorders with International Participation. The Therapy of Stress Related Disorders, Rabac, Croatia, June 5-7, 2008.

17. Pivac N, Nedić G, Deželjin M, Mustapić M, Mimica N, Muck-Šeler D, Folnegović-Šmalc V. Catechol-o-methyl-transferase val158/met polymorphism in Alzheimer's Disease. 4th Croatian Congress on Alzheimer's Disease with International Participation, Rovinj, Croatia, October 8-11, 2008.
18. Pivac N, Nedić G, Mustapić M, Muck-Šeler D, Kozarić-Kovačić D. Biological background and pharmacotherapy of psychotic posttraumatic stress disorder. Third Regional CINP Congress, Bratislava, Slovakia, November 27-30, 2008.
19. Žarković N: Development and Validation of New Technologies for Faster Analysis, Bioanalysis in Clinical Research, Post Conference Workshop, Olympia Conference Centre, London, UK, February 22, 2008.
20. Žarković N: ELISAs in LPO detection, Free Radicals and Nutrition: basic mechanisms and clinical applications, SFRR Europe & COST B35 Action, Berlin, Germany, July 5-9, 2008.
21. Žarković N: Lipid Peroxidation Associated Diseases, COST Outreach Activity for Early Stage Researchers in connection with Euro Science Open Forum, Barcelona, Spain, July 19, 2008.
22. Žarković N: The Relevance of Immunochemistry of 4-Hydroxy-2-nonenal for Evaluation of its Biological Activities, Lipid Peroxidation 2008, Karuizawa, Japan, October 15-17, 2008.
23. Pavelić K.: The role of integrative genomics/proteomics in the detection and treatment of metastatic breast cancer. 5th Conference on Experimental and Translational Oncology. Kranjska Gora, Slovenia, March 26-30, 2008.
24. Pavelić K, Varela-Nieto I.: Stem cells and tissue engineering. European Medical Research Council Forward Look. EMRC 52nd Plenary meeting. The Royal College of Physicians. London, UK, April 22-23, 2008.
25. Pavelić K.: Improved navigation and precise drug delivery (contributed talk). HotNanoTopics. Nanostructured bio-interfaces. Portorož, Slovenia, May 26-30, 2008.
26. Pavelić K.: Casting light on molecular events underlying metastasis of cancer: what can be

seen from the -omics point of view. 38th Annual meeting of European Environmental Mutagen Society (EEMS) Cavtat, Croatia, September 21-25, 2008.

27. Pavelić K.: Presentation of the ESF-EMRC Science Policy Briefing on stem cell research. European Science Foundation, European Medical Research Council. Paris, France, October 13, 2008.

SELECTED PUBLICATIONS

Research articles

1. Antica M, Čičin-Šain L, Kapitanović S, Matulić M, Džebro S, Dominis M. Aberrant ikaros, aios and helios expression in Hodgkin and non-Hodgkin lymphoma. *Blood* 2008; 6: 3296.
2. Čačev T, Radošević S, Križanac Š, Kapitanović S. Influence of interleukin-8 and interleukin-10 on sporadic colon cancer development and progression. *Carcinogenesis* 2008; 29:1572.
3. Čipak A, Jaganjac M, Tehlivets O, Kohlwein SD, Žarković N: Adaptation to oxidative stress induced by polyunsaturated fatty acids in yeast. *Biochim. Biophys. Acta Mol. Cell Biol Lipids* 2008;178: 283.
4. Grbeša I, Marinković M, Ivkić M, Krušlin B, Novak Kujundžić R, Pegan B, Bogdanović O, Bedeković V, Gall Trošelj K. Loss of imprinting of IGF2 and H19, loss of heterozygosity of IGF2R and CTCF, and *Helicobacter pylori* infection in laryngeal squamous cell carcinoma. *J Mol Med JMM* 2008; 86: 1057.
5. Hranjec M, Piantanida I, Kralj M, Šuman, L, Pavelić K, Karminski-Zamola G. Novel amidino-substituted thienyl- and furyl-vinyl-benzimidazole derivatives and their photochemical conversion into corresponding diaza-cyclopenta[c]fluorenes. Synthesis, interactions with DNA and RNA and antitumor evaluation. *J Med Chem* 2008; 51: 4899.
6. Jaganjac M, Poljak-Blaži M, Žarković K, Joerg Schaur R, Žarković N. The involvement of granulocytes in spontaneous regression of Walker 256 carcinoma. *Cancer Let* 2008; 260: 180.
7. Kraljević Pavelić S, Čačev T, Kralj M. A dual role of p21^{waf1/cip1} gene in apoptosis of HEP-2 treated with cisplatin or methotrexate. *Cancer Gene Ther.* 2008; 15: 576.

8. Novak Kujundžić R, Grbeša I, Ivkić M, Katdare M, Gall Trošelj K. Curcumin downregulates H19 gene transcription in tumor cells. *J Cell Biochem* 2008; 104: 1781.
9. Sabol I, Salakova M, Smahelova J, Pawlita M, Schmitt M, Gasperov NM, Grce M, Tachezy R. Evaluation of different techniques for identification of human papillomavirus types of low prevalence. *J Clin Microbiol* 2008; 46 :1606.
10. Sedić M, Poznić M, Gehring P, Scott M, Schlapbach R, Hranjec M, Karminski-Zamola G, Pavelić K, Kraljević Pavelić S. Differential antiproliferative mechanisms of novel derivative of benzimidazol-1,2- α -quinoline in colon cancer cells depending on their p53 status. *Mol Cancer Ther* 2008; 7: 2121.
11. Sobočanec S, Balog T, Kušić B, Šverko V, Šarić A, Marotti T. Differential response to lipid peroxidation in male and female mice with age: correlation of antioxidant enzymes matters. *Biogerontology* 2008; 9: 335.
12. Šagud M, Pivac N, Nedić G, Mihaljević Peleš A, Kramarić M, Jakovljević M, Muck Šeler D. The effect of lamotrigine on platelet serotonin concentration in patients with bipolar depression. Letter to the editors. *Psychopharmacology* 2008; 4: 683.

Review articles

1. Bošnjak H., Pavelic K., Kraljevic Pavelic S.: Towards preventive medicine. High-throughput methods from molecular biology are about to change daily clinical practice. *EMBO Rep* 2008; 9: 1056.
2. Grce M, Davies P. Human papillomavirus testing for primary cervical cancer screening. *Expert Rev Mol Diagn* 2008; 8: 599.
3. Kralj M, Tušek-Božić Lj, Frkanec L. Biomedical Potentials of Crown Ethers: Prospective Antitumor Agents. *ChemMedChem*. 2008; 3: 1478.
4. Levanat S, Čretnik M, Musani V. Hh-Gli signaling pathway functions and its therapeutic potential in cancer , *Croatica Chemica Acta* 2008; 81: 1.
5. Šagud M, Mihaljević-Peleš A, Pivac N, Muck-Šeler D, Šimunović I, Jakovljević M: Genetics of schizophrenia in the context of integrative psychiatry. *Psychiatria Danubina* 2008; 20: 364.

Chapters in books

1. Borović Šunjić S, Šunjić I, Wildburger R, Mittelbach M, Waeg G, Žarković N: Lipid peroxidation end product as a modulator of cell growth. In: *Cell Growth Processes: New Research*. Nova Science Publishers, Inc. Hayashi T (Ed) New York, 2008: 187
2. Pivac N, Kozarić-Kovačić D, Nedić G, Mustapić M, Stipčević T, Nenadić-Šviglin K, Grubišić-Ilić M, Mück-Šeler D. Neurobiology of Suicidal Behaviour. In: *Wounds of War: Lowering Suicide Risk in Returning Troops*. NATO Science through peace and security – Editor: Wiederhold, Brenda K. IOS Press Amsterdam, 2008, pp 3-22.
3. Sobočanec S, Šarić A, Korolija M, Marjanović M, Kralj M, Knežević J, Čretnik M, Balog T, Šverko V, Kušić B, Marotti T. Native propolis in vivo: On the oxidative/antioxidative effect and the mechanism of action. In: *Scientific Evidence of the Use of Propolis in Ethnomedicine*- Editor:Transworld Research Network Fort P.O., Kerala, India, 2008, pp 121-131.

Books

1. Boranić M et al. (Balog T, Čurić G, Gabrilovac J, Gregurek R, Koršić M, Lauc G, Marotti T, Martin Kleiner I, Pivac N, Muck-Šeler D, Sabioncello A, Stojević Z, Trkulja V) *Psychoneuroendocrinology: interaction of immune, nervous and endocrine systems (Psihoneuroimunologija: povezanost imunosustava sa živčanim i endokrinim sustavom)*. Editor: Krznarić Vohalski G. Školska knjiga dd. Zagreb, 2008, pp 1-277.
2. Pivac N, Kozarić-Kovačić D, Mustapić M, Deželjin M, Nenadić-Šviglin K, Muck-Šeler D. Peripheral biological markers in alcoholism. Editor: Pivac N. New York, Nova Publishers, 2008, pp 1-93.
3. Duraković Z, Žarković N: Biology of aging and geriatry (Biologija starenja i gerijatrija) In: Vrhovec B et al., *Internal Medicine (Interna medicina)*, Editor: Vrhovec B, Naklada Ljevak, Zagreb, pp 69-77.



Division of Marine and Environmental Research

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

OMIZ

DIVISIONAL ORGANIZATION

Head: Tarzan Legović

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

- ⇒ Informatics and environmental modelling, Tarzan Legović
- ⇒ Satellite oceanography, Milivoj Kuzmić
- ⇒ Aquatic physical chemistry, Zlatica Kozarac
- ⇒ Physical chemistry of traces, Milivoj Lovrić
- ⇒ Colloid geochemistry, Ivan Sondi
- ⇒ Inorganic environmental geochemistry, Goran Kniewald
- ⇒ Bioelectrochemistry and surface imaging, Vesna Svetličić
- ⇒ Analytical chemistry and biogeochemistry of organic compounds, Marijan Ahel
- ⇒ Radioecology, Delko Barišić
- ⇒ Biological effects of metals, Biserka Raspor
- ⇒ Molecular ecotoxicology, Tvrtko Smital
- ⇒ Aquaculture and pathology of aquatic organisms, Emin Teskeredžić



OVERVIEW OF THE DIVISION

During 2008, division scientists worked on more than 50 research projects contracted by the Ministry of Sciences, Sport and Education and outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from satellite oceanography down to nano-technology. Each project contributed to the overall mission of the division, which is to strive for excellence in fundamental and applied research of environmental systems, their processes, states and control. The research is directed toward an increase in the knowledge base needed for the optimum management of the environment and hence to the benefit of our country and, indeed, the whole world.

The research results were published in 53 scientific papers in journals indexed by Current Contents, one patent received favourable reports internationally, three books were published, 5 invited lectures were held and 5 conferences were organized. In addition, 4 graduate schools were coordinated,

2 B.Sc, 2 M.Sc. and 4 Ph.D. theses were defended, under the mentorship of Division scientists. Finally, 18 undergraduate and 63 post-graduate courses were given at universities in Croatia and abroad.



Figure 1. Single quadrupole GC/MS system installed in the Laboratory for Biogeochemistry of Organic Compounds.

TOP ACHIEVEMENTS

Overfishing of predatory benthic fishes in the Adriatic Sea confirmed

It has been shown that most of the predatory benthic fish stocks in the Adriatic Sea have been overfished. Observed changes between populations of Chondrichthyes and Osteichthyes are in agreement with the Volterra principle down to the extinction of predators. By using the Gause competition model under the intensive fishery, it is shown that an initially dominant competitor may become marginal, in agreement with existing data. These alarming results indicate the need for a new approach to the management of the multispecies fisheries (Legović, 2008).

A novel biomimetic nano-scale aggregation route

A novel, bio-inspired precipitation strategy, determined as *biomimetic nano-scale aggregation route*, in formation of nanostructured submicron-size colloidal particles of carbonates was described. It involves simultaneous inhibitory effect of magnesium ions

on the crystal growth of initially formed nanocrystallites of calcite and subsequent aggregation processes of these particles that govern the formation of submicron size and nanostructured hierarchical structures of colloidal carbonates. This finding is relevant in understanding the mechanism of formation of complex natural hybrid materials, found in bioinorganic structures generated through nanoparticle assemblies (Sondi et al., 2008).

A novel approach in the determination of trace metal – natural organic matter interactions

An adapted protocol for the electrochemical characterization of the metal ion - natural organic matter (NOM) interaction is proposed and tested. A realistic speciation of metal ions in the particular natural water, derived from the calculated complexing parameters is obtained (Loius et al., 2008).

Passive samplers for metals applied as a new tool

Passive samplers, DGTs (diffusive gradients in thin films), were applied in the Sava River water (Croatia) as a new tool for the assessment of the labile metal concentrations. Increased concentrations of Co, Cr, Mn and Fe were found at the location downstream of the municipal sewage outlet, indicating a detrimental effect of the pollution point source on surface water quality (Dragun et al., 2008).

The evidence of self-purification of the Krka River

This study provides the first survey of trace metal content in the Krka River using 'clean' methods and techniques of sampling, handling and analysis. Concentrations of Zn, Cd, Pb and Cu measured in the water of the Krka River are amongst the lowest reported in the literature for freshwater systems (Cukrov et al., 2008).

Anchialine cave-waters – evidence for sustained localised oxidation of iodide to iodate

Anchialine caves provide unusual environmental conditions due to lack of light, relatively long seawater residence time, hypoxia, and an exacerbated role of bacteria in the food-web. The caves in Croatia provide interesting iodine chemistry with iodide oxidation in bottom waters, iodate reduction and iodide remineralization in mid-water, at the halocline. Anchialine caves offer an opportunity to improve the understanding of the biogeochemical mechanisms operating generally with iodine in marine systems (Žic et al., 2008).

Total mercury in core sediments in the Bay of Bengal, India

The concentration of total mercury in core sediments (<63 μm) of Sunderban mangrove wetland, the Bay of Bengal varies from 9.8 to 535.1 ppb (ngg^{-1}). Based on Igeo and RE-L (150 ppb) it is concluded that sediments are unpolluted. Two statistical methods were applied to determine Hg anomalies at post monsoon and in pre monsoon period. Results will be useful in future sediment quality studies (Kwok et al., 2008).

Magnetic susceptibility of coal combustion products in sediments

Coal slag and ash, obtained from burning coal in a textile factory in Duga Resa (Croatia), have been discharged directly into the Mrežnica River for 110 years. The effects have spread almost to Karlovac, 50 km downstream from the source. Cluster analysis of R-modality indicates that low-field magnetic susceptibility (MS) is linked to B, Mo, Na and U (Frančišković-Bilinski, 2008).

Study of organic complexation in atmospheric precipitation

Organic complexation in atmospheric precipitation is an important control mecha-

nism of the biogeochemistry of metal ions. Complexation of copper ions in bulk precipitation was measured using differential pulse anodic stripping voltammetry (DPASV). The precipitation samples were collected periodically during one year in the mainland area of Croatia (Zagreb) and at the Adriatic coast (Šibenik). The complexation of copper ions ranges from 0.010 and 1.4 μM . The highest capacity was measured in April 2003 in a rainwater sample from the Šibenik area (Plavšić et al., 2008).

Accumulation mechanism for metal chalcogenide nanoparticles at Hg electrodes

Mercury electrodes preconcentrate metal chalcogenide nanoparticles, enabling their detection at submicromolar concentrations by adsorptive cathodic stripping voltammetry. A multistep mechanism was proposed with polydisperse copper sulphide (Cu_xS) nanoparticles. Particles obey the Schulze-Hardy rule at various electrolyte strengths and, consequently, accumulation rates are strongly sensitive to electrolyte concentrations (Krznařić et al., 2008).

Fish cells can develop the multi-drug/multixenobiotic resistance phenotype similar to mammalian tumour cells

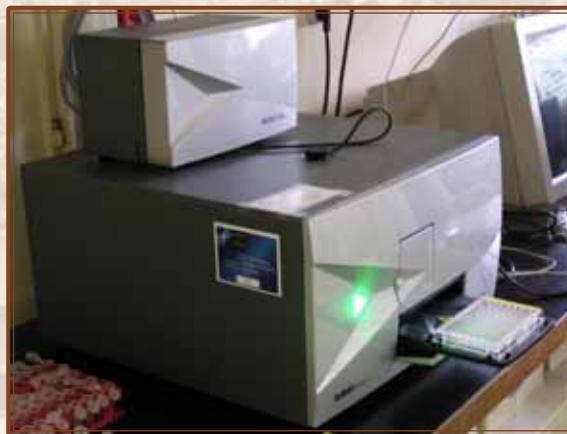


Figure 2. TECAN Infinite M200 system installed in the Laboratory for Molecular Ecotoxicology.

It is demonstrated that fish PLHC-1/dox cells highly express P-glycoprotein (ABCB1) mediated multidrug resistance, exhibiting similar cross-resistance phenotype to structurally different xenobiotics as the one described in mammalian cells. This finding affirms the PLHC-1 cell line as an important model for studying the development of basic resistance mechanisms to different chemicals in aquatic organisms (Žaja et al., 2008).

Fish health status in relation to water quality

Freshwater fish are monitored on a regular basis in several Croatian rivers (Sava, Kupa, Dobra, Mrežnica, Zrmanja, Krka and Sutla). Investigations of biochemical parameters, resorption of nutrients, occurrence of bacterial, viral and parasitic diseases as well as the aquaculture technology and cultured fish diet have been carried out. Since water quality is the main factor affecting aquaculture, fish could be used as probes of the water quality. In addition, our goal is to detect the impact of wild populations as a reservoir of pathogens (Kapetanović et al., 2008).

Occurrence and fate of pharmaceuticals in wastewaters and natural waters

A comprehensive reconnaissance of over seventy individual contaminants in Croatian municipal wastewaters was performed, including some prominent classes of emerging contaminants such as pharmaceuticals and personal care products, surfactants and their degradation products, plasticizers, pesticides, insect repellents, and flame retardants. Due to the rather poor wastewater management practices, most of the contaminants present in wastewaters reach ambient waters and may represent a significant environmental concern (Terzić et al., 2008).

PATENT

Hršak D, Havriluk M. Mixed bacterial culture for atrazine degradation, WO 2007/0966681 A1. The patent application obtained excellent international search report and entered into national phases in EU, USA, India, China, Canada and Australia.

New equipment

TECAN Infinite M200 modular monochromator-based microplate detection system with fluorescence, absorbance and luminescence detection modes is being used for determination of intracellular accumulation or efflux of model compounds in a variety of (eco) toxicologically relevant bioassays (Smital T).

GC/MS system with EI, positive and negative CI, Agilent 7890A Series GC and 5975B inert XL MSD is being used for the determination of specific organic contaminants in various environmental matrices (Ahel M).

Ultra performance Liquid Chromatography/Quadrupole-Time-of-Flight Mass Spectrometry (UPLC/Q-ToF), Waters UPLC/Q-ToF Premier is being used for the determination of polar environmental pollutants. The major advantage is the capability of the instrument to measure mass accurately, which provides the basis for identification of unknown contaminants in complex environmental matrices (Terzić S).



Figure 3. Biomimetic formation of nanoscale colloidal carbonates in the Laboratory for colloid geochemistry.

The Beckman Coulter LS 13320 is the most versatile multi-wavelength laser diffraction particle size analyzer available today. Depending on applications and requirements, it produces reliable results on particle sizing for aqueous and non-aqueous samples and dry powders in the range from 20 nm to 2 mm (Sondi I).

EDUCATION

Four graduate school studies were coordinated by the Division members. This includes: studies on Biophysics with the University of Split, Environmental Management and Oceanography with the University of Zagreb, and Environmental Protection and Nature Conservation with the University J.J. Strossmayer in Osijek.

HONOURS AND AWARDS

Mirčeski V, Komorsky-Lovrić Š, and Lovrić M were awarded Macedonian State Award "Goce Delčev", 2008, for the book "Square-Wave Voltammetry. Theory and Application", Springer, Berlin, 2007.

Sondi I was awarded The Croatian Academy of Sciences and Arts prize for the highest scientific achievement in natural sciences in Croatia.

Sondi I was awarded The Scientific Excellence Award, from the Croatian Ministry of Sciences, Education and Sports for the highly cited article published in Journal of Colloid and Interface Science (2004) 275, 177-182.

PROJECTS AND PROGRAMS

Research projects supported by the Ministry of Sciences, Education and Sports

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

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

Program supported by the Ministry of Sciences, Education and Sports

1. Biogeochemical processes and environmental risk, Marijan Ahel

Selected research, developmental and international projects

1. A complex study of marine organic matter characterization in seas of the European coastal zone, Blaženka Gašparović (Bilateral collaboration with Alfred Wegener Inst Polar & Marine Res, Bremerhaven, Germany).
2. AFM study of the crystallization of synthesized zeolites, Vesna Svetličić (Bilateral Co-

- operation, Eötvös Loránd University, Budapest, Hungary)
3. Biogeochemical processes in anoxic environments: electrochemistry as an alternative tool for trace metals and sulphur determination, Irena Ciglencečki-Jušić (Bilateral collaboration with Eötvös Loránd University, Budapest, Hungary)
 4. Characterization of river sediment contamination from humid tropical Hugli River, India and temperate rivers of Croatia in terms of geochemical and mineralogical data based on weathering, Halka Bilinski (Indian-Croatian bilateral cooperation)
 5. Comparative study between the anthropogenically impacted coastal area of Shanghai (China) and the pristine environment of the Krka river estuary (Croatia), Goran Kniewald (Bilateral cooperation with East China Normal University, Shanghai, China)
 6. Developmental program for expert basis and studies in freshwater fisheries in 2008, Group A – fisheries area Kupa, Emin Teskeredžić (project financed by the Ministry of Agriculture, Fisheries and Rural Development)
 7. Direct determination of arsenic species in natural ecosystems by electrochemistry and modelling of its speciation, Dario Omanović (ECO-NET, French-Croatian-Bosnian cooperation project)
 8. Ecosystem Approach for Sustainable Aquaculture, Tarzan Legović (EU-FP6).
 9. Assessment of hazardous chemical contamination in the Sava River basin, Marijan Ahel and Tvrtko Smital (NATO Science for Piece)
 10. Electrochemical characterization of marine polysaccharides, Marta Plavšić (Deutsche Forschungsgemeinschaft)
 11. Environmental impact assessment of the Mandalina marine, Neven Cukrov, Željko Kwokal, Tarzan Legović (NCP Nautic Centre Prgin)
 12. Environmental impact assessment of the mineral fertilizer factory in Vukovar, Tarzan Legović and B. Hackenberger (Adriatica Dunav)
 13. Evaluation of contamination of stream sediments in lithologically different drainage basins, using advanced geomathematical methods, Stanislav Frančišković-Bilinski (Austrian-Croatian bilateral cooperation)
 14. Highly specific determination of illicit drugs in municipal wastewater as a basis for the assessment of the drug abuse trends in the City of Zagreb, Senka Terzić (City of Zagreb)
 15. Impact of fish farms on marine ecosystems of the Adriatic Sea, Goran Kniewald (Croatian-Slovenian bilateral cooperation)
 16. Marine science and coastal management in the Adriatic Western Balkan, An education and research network, Božena Čosović, (Norwegian cooperation programme on research and higher education)
 17. Mechanism of mucilage formation in the Northern Adriatic Sea, Vera Žutić (Bilateral Cooperation with NSF, USA, Scripps Institution of Oceanography)
 18. Monitoring of freshwater fisheries in 2008, Group D – fisheries area Sava; River Sutla, Emin Teskeredžić (Ministry of Agriculture, Fisheries and Rural Development)
 19. Novel physical chemical techniques to characterize the sea surface microlayer, Zlatica Kozarac (UK Royal Society)
 20. On line toxicity sensors based on modification of membrane organisation, Blaženka Gašparović (NATO, Science for peace and security programme)
 21. Radiological monitoring around Nuclear Power Plant Krško, Željko Grahek (Krško NPP, Slovenia)
 22. Radiological Monitoring of Danube River, Delko Barišić (Croatian Waters Management)
 23. Reference Laboratory, Božena Čosović, Dubravka Hršak, Zlatica Kozarac, Biserka Raspor (Project funded through the Ministry of Regional Development, Forestry and Water Management, Water Management Directorate)
 24. Regular research of radioactivity in marine indicator organisms, Delko Barišić (State office for radiation protection)
 25. Research of biological and physico-chemical parameters in the Vrana Lake, Emin Teskeredžić (potable water reservoir, island Cres).

ORGANIZED CONFERENCES

1. 1st Regional Symposium on Electrochemistry for South-East Europe (RSE-SEE), May 4-8, 2008. Crveni otok, Rovinj, Croatia, Horvat-Radošević, V.
2. 7th Symposium of Croatian Radiation Protection Association May 29-31, 2008, Opatija, Croatia, Grahek, Ž. and Barišić, D.
3. Second Annual Meeting in Albania of the Project "Marine science and coastal man-

agement in the Adriatic, Western Balkan. An education and research network", Durrresi, Albania, September 29 – October 3, 2008, Čosović, B. and Wassman, P.

4. First Regional Symposium on Electrochemistry of South-East Europe, Rovinj, Croatia, May 4-8, 2008. Ivošević DeNardis N.
5. 3rd Christmas Biophysics Workshop: Organized Molecular Systems, Donja Stubica, Croatia, December 15-16 2008, Svetličić, V.

INVITED LECTURES

1. Ahel, M. Surfactants and surfactant metabolites in wastewaters and ambient waters, International Conference on Environmental Research and Mitigation of Water Pollution in Romania and in the Lower Danube Region, Bucharest, Romania, September 3-5 2008.
2. Svetličić, V. Mucilage phenomenon at the nanoscale. Faculty of Natural Sciences, University of Split, October 7 2008.
3. Ciglencečki, I., Bura-Nakić, E., Carić, M., Kršinić, F., Viličić, D., Burić, Z., Čosović, B. Seasonal variation of oxic-anoxic conditions in the small, seawater lake (Rogoznica Lake, East Adriatic Coast) related to the global climate changes. Regional Process of the 5th World Water : Water in the Mediterranean Basin, Near East University, Lefkosa, TRNC, October 8-10, 2008.
4. Legović, T. Future of marine resources management. Regional process of the 5th World Water Forum: Water in the Mediterranean Basin Near East University, Lefkosa, TRNC, October 8-10, 2008.



Figure 4. Male spawner Brown Trout (*Salmo trutta fario*) from "Krčić", Knin, fish farm.

5. Kuzmić, M. Exploring the Adriatic Bora-induced motions: Observations & Modelling, DZLR, Oberpfaffenhofen, Wessling, Germany, November 11, 2008.

SELECTED PUBLICATIONS

Books

1. Komarov S. and Legović T. (Eds.) The fifth European Ecological Modelling Conference, Ecological Modelling, Elsevier, pp. 1-177, 212, 2008.
2. Barišić, D., Grahek, Ž., Krajcar Bronić, I. and Miljanić, S. (Eds) Proceedings of the 7th Symposium of Croatian Radiation Protection Association. RBI, Zagreb, Croatia. 2008.
3. Deza, M. and Dutour Sikirić, M. Geometry of Graphs, Polycycles and Two-faced Maps, Series: Encyclopaedia of Mathematics and its Applications No. 119, ISBN-13: 9780521873079, Cambridge University Press, 2008.

Scientific papers

1. Cukrov N, Cmuk P, Mlakar M, Omanović D. Spatial distribution of trace metals in the Krka River, Croatia. An example of the self-purification. Chemosphere 2008: 72: 1559.
2. Dragun Z, Raspor B, Roje V. The labile metal concentrations in Sava River water assessed by diffusive gradients in thin films. Chem Speciation Bioavailability 2008: 20: 33.
3. Frančišković-Bilinski S. Detection of geochemical anomalies in stream sediments of the upper Sava River drainage basin (Slovenia, Croatia). Fresenius Environmental Bulletin 2008: 17: 188.
4. Gašparović B, Frka S, Kozarac Z, Nelson A. A method for characterization of sea surface microlayer based on monolayer properties in presence and absence of phospholipids. Anal Chim Acta 2008: 620: 64.
5. Kapetanović D, Vardić I, Kurtović B, Valić D, Teskeredžić E. Detection of the causative agent of furunculosis, *Aeromonas salmonicida* in salmonids of the Krka River. Vet Res Commun 2008: 32: 131.
6. Krznarić D, Helz GR, Bura-Nakić E, Jurašin D. Accumulation mechanism for metal chalcogenide nanoparticles at Hg electrodes: Cu sulphide example. Anal Chem 2008: 80: 742.

7. Kwokal Ž, Sarkar SK, Chatterjee M, Frančišković-Bilinski S, Bilinski H, Bhattacharya AK, Bhattacharya BD, Aftab A. An Assessment of Mercury Loading in Core Sediments of Sunderban Mangrove Wetland, India (A Preliminary Report). *Bull Environ Contam Toxicol* 2008: 81: 105.
8. Legović T. Adriatic Sea: Impact of the demersal fishery and evidence of the Volterra principle to the extreme. *Ecol modelling* 2008: 212: 68.
9. Louis Y, Cmok P, Omanović D, Garnier C, Lenoble V, Mounier S, Pižeta I. Speciation of trace metals in natural waters: The influence of an adsorbed layer of natural organic matter (NOM) on voltammetric behaviour of copper. *Anal Chim Acta* 2008: 606: 37.
10. Plavšić M, Orlović-Leko P, Kozarac Z, Bura-Nakić E, Strmečki S, Čosović B. Complexation of copper ions in atmospheric precipitation in Croatia. *Atmospheric Res* 2008:87:80.
11. Sondi I, Škapin SD, Salopek-Sondi B. Biomimetic precipitation of nanostructured colloidal calcite particles by enzyme-catalyzed reaction in the presence of magnesium ions. *Cryst Growth Des* 2008: 8: 435.
12. Terzić S, Senta I, Ahel M, Gros M, Petrović M, Barcelo D, Muller J, Knepper T, Marti I, Ventura F, Jovančić P, Jabučar D. Occurrence and fate of emerging wastewater contaminants in Western Balkan Region. *Sci Total Environ* 2008: 399: 66.
13. Udiković Kolić N, Martin-Laurent F, Devers M, Petrić I, Begonja Kolar A, Hršak D. Genetic potential, diversity and activity of an atrazine-degrading community enriched from a herbicide factory effluent. *J Appl Microbiol* 2008: 105: 1334.
14. Žaja R, Caminada D, Lončar J, Fent K, Smital T. Development and characterization of P-glycoprotein 1 (Pgp1 ; ABCB1) mediated doxorubicin-resistant PLHC-1 hepatoma fish cell line. *Toxicol Appl Pharmacol* 2008: 227: 207.
15. Žic V, Truesdale VW, Cukrov N. The distribution of iodide and iodate in anchialine cave-waters – evidence for sustained localised oxidation of iodide to iodate in marine water, *Mar Chem* 2008: 112: 168.

Chapters in books

1. Legović, T. Mathematical Ecology. In: *Encyclopedia of Ecology*, Jørgensen, S.E. and Fath, B.D. (Eds). Elsevier, 2008, pp 2261-2266.
2. Smital, T. (2008) Acute and Chronic Effects of Emerging Contaminants. In: *The handbook of environmental chemistry -Emerging Contaminants from Industrial and Municipal Wastewaters*. Barcelo, D. & Petrović, M. (Eds.), Springer-Verlag, Heidelberg, Germany, 2008, pp 105-142.

Centre for Marine Research

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

DIVISIONAL ORGANISATION

Head: Nenad Smodlaka

The Centre for Marine Research consists of the following laboratories:

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



OVERVIEW OF THE DIVISION

The mission of the Centre for Marine Research is the study of the processes in the marine environment from sub cellular to regional scale, especially in benthic communities and the water column. Other than basic research, the Centre is involved in monitoring of the Adriatic Sea for the government purposes and several international projects (Interreg) regarding protection of the marine environment.

TOP ACHIEVEMENTS

Drastic recent changes in the northern Adriatic ecosystem

Historical data sets of physical, chemical and biological oceanographic parameters, collected since 1965 at 16 stations located between the Rovinj waters (western Istria,

Croatia) and the zone 12 Nm off the Po River delta (Italy), have been analysed. The salinity of the upper water column was markedly higher in the period 1998-2007, compared to the previous one (1972-1997), particularly since 2003. This was mainly correlated with an extremely low Po River water discharge in 2005 and 2007. Consequently, a significant reduction of orthophosphate and orthosilicate concentrations in the investigated region occurred, causing a decrease of the phytoplankton biomass, primarily of the nano fraction, as well as of the chlorophyll *a* concentration. Concurrently, the water transparency increased. However, the nitrate concentration increased in the sea, in spite of its lower riverine contribution. This can be attributed to an enhanced accumulation of the unused fraction in the primary production processes. In fact, the N/P ratio in the Po River water is very high and it increased more significantly since the late eighties after a 2.5 fold reduction of the phosphorus concentration. It was mainly due to the ban of polyphosphates in detergents. The observed changes are probably partially related to climatic fluctuations, characterized by longer periods of dry weather in the last 20 years, and at least in part to the anthropogenic global warming.

Alkaline phosphatase activity in relation to the nutrient status in the northern Adriatic

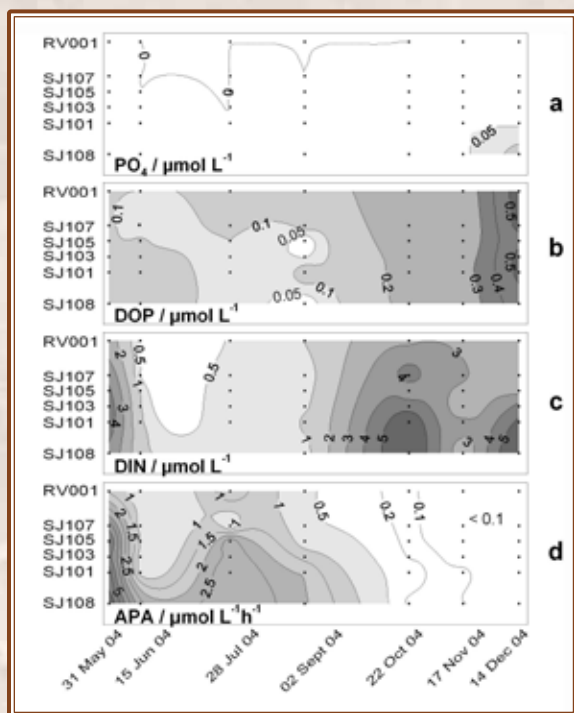


Figure 1. PO₄ (a), DOP (b), DIN (c), and APA (d) distributions at the surface during 2004.

The role of APA in meeting the seasonal microbial phosphorus requirements in the northern Adriatic, an area poor in orthophosphate (PO₄), was emphasized. From May to September, in conditions of exhausted PO₄, microbes in upper waters induced high APA (0.41–5.55 μmol L⁻¹ h⁻¹) to obtain phosphorus from the dissolved organic pool. The highest APA was found during spring and summer freshets due to the strongly deficient PO₄ versus inorganic nitrogen supply from the Po River. During summer months APA was lower, yet still important for phosphorus recycling, although a low Po River nitrogen supply resulted in lower microbial biomass and consequently in lower APA as well. From October to December APA in upper waters was low (<0.2 μmol L⁻¹ h⁻¹), even during large microbial blooms, when PO₄ was probably supplied from deeper waters. APA was generally irrelevant in deeper waters due to

an almost balanced inorganic N/P ratio for microbial requirements.

Caulerpa racemosa: Adaptive varieties studied by fatty acid composition

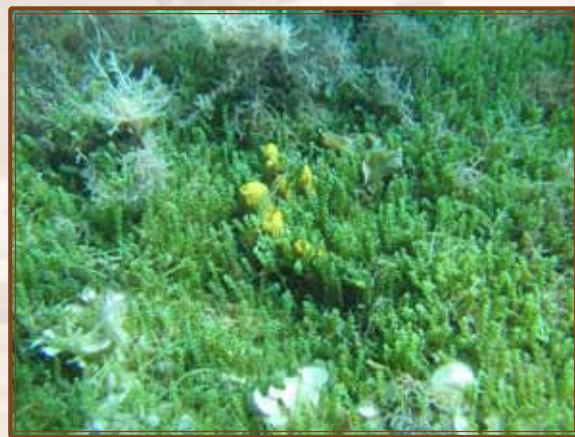


Figure 2. *C. racemosa* meadow along the coast of St. Juraj isle.

Total lipids and fatty acid composition were monitored seasonally in exposed and sheltered *Caulerpa racemosa* settlements along the coast of St. Juraj isle (Vrsar, Croatia). Despite the proximities of both populations studied, which implies a similar level exposure to seasonal fluctuations, the alga responses were different. Total lipid changes and fatty acid composition of the related settlements indicated the differences in thalli condition during summer and, to some extent, different strategies in cold adaptation during winter. In August the bad condition of thalli at the sheltered site expressed by low unsaturation (UNS/SAT 0.45) resulted from its sexual propagation state, in contrast to the advanced condition of vegetative propagation state at the exposed site (UNS/SAT: 1.1). The poor thalli condition was related to its slower development at the sheltered habitat, having correspondingly a lower biomass. At this site little to no difference in total lipids was observed with season. During the winter period (min. temp. 7.7 °C) both settlements altered their fatty acid composition by increasing unsaturation (UNS/SAT up to 1.8), but a pronounced win-

ter peak in total lipids occurred at the exposed site. Under similar environmental conditions, *C. racemosa* developed different strategies in cold adaptation and propagation state as a consequence of apparently varying impact of the hydrodynamism at these two proximate sites. This study suggests the mode in which exposure impacts the growth cycle of *C. racemosa* in temperate regions.

Phototrophic pico- and nanoplankton communities in the northern Adriatic

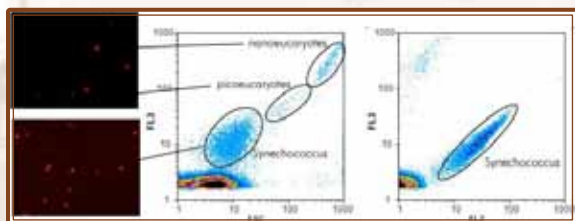


Figure 3. 2-D diagram of phototrophic pico- and nanoplankton cells.

Flow cytometric analysis reveals a more complete estimation of abundance and biomass of all major groups of pico- and nanophototrophs in this area than has been available until now, allowing thus a better insight into their potential relative importance both as producers and prey. The first records of *Prochlorococcus* were obtained. *Synechococcus* were the most abundant phototrophs in the area, occasionally matched in number by previously rarely studied phototrophic picoeukaryotes. In terms of biomass, the latter usually comprised more than 50 % of the phototrophic pico-biomass, sometimes up to 90 %. The under-researched phototrophic picoeukaryotes thus seem to be much more important for this ecosystem than was previously thought, while preliminary results on the presence of *Prochlorococcus* indicate their minor importance in this hydrologically and biologically dynamic area. Estimations of the contribution of each size fraction in the total phototrophic biomass (pico-, nano- and micro-) reveal higher portions of pico- and nano- fraction on average compared to micro-fraction.

Alien bivalve species in the northern Adriatic Sea

All but one species of the family Pteriidae (Bivalvia, Pterioidea) reported so far from the Mediterranean Sea are introduced to the Mediterranean either via the Suez Channel (*Pinctada radiata*, *Pteria occa*), by aquaculture activities (*Pinctada margaritifera*, *P. radiata*) or via shipping (*Electroma vexillum*). A few specimens of the lessepsian bivalve *P. radiata* were encountered in the northern Adriatic offshore waters (silty-sand bottom, 59 m depth). That was the first record of the species in the Croatian part of Adriatic Sea (Doğan and Nerlović, 2008).

Colonization patterns of the date mussel on artificial structures

A colonization pattern of the date mussel on limestone breakwater boulders, which have been placed for 19 years along the dike of the Rovinj Marina, were studied and compared with natural habitats. In distinction



Figure 4. Date mussels' boreholes on a breakwater boulder of the marina of Rovinj. In sheltered habitats, 19 years after the placement of boulders in the sea, density and total biomass of date mussels were around 800 individuals m^{-2} and 3.5 $kg\ m^{-2}$, respectively.

from natural habitats, an unexpected high colonization rate and growth of date mussels was detected on certain unexposed break-water boulders so the results could be useful in predicting the reconstruction of natural populations of the date mussel after harvesting (Devescovi and Iveša, 2008).

Ecology and distribution of the sponge *Aplysina aerophoba* in Limski kanal

Information about sponge distribution patterns and their dependence on light, depth, substrate and other factors could be very useful for *in situ* culture and can be utilized to improve *in vitro* maintenance conditions, because a sustainable growth has not yet been observed *ex situ*. An observed decrease of abundance and size of *A. aerophoba* along a depth gradient can be explained with shading by rocky notches close to the water surface, by the presence of benthic competitors (mainly algae) or by high sedimentation which increases towards the eastern end of the bay (Zucht et al., 2008).

Shell biominerals, enzymatic activity and shell matrix proteins

In the last few years, the field of molluscan biomineralization has undergone a tremendous conceptual transformation. Recent advances deal more particularly with the structure of shell biominerals at the nano-scale, and with the identification of an increasing number of shell matrix protein components. In this review different aspects of the molluscan shell, from evolutionary and from mechanistic viewpoints, are described (Marin et al., 2008).

The role of alkaline phosphatase

The role of alkaline phosphatase in meeting the seasonal marine microbial phosphorus requirements of the northern Adriatic has

been quantified in detail for the first time for the northern Adriatic (Ivančić et al., 2008). It has been discovered that alkaline phosphatase plays a vital role in marine microbial communities' phosphorus recycling in this orthophosphate-poor area.

The effects of hypo-osmotic stress

The effects of hypo-osmotic stress on biological parameters in marine molluscs have been employed as a useful tool in pollution assessment. The progressive acclimation of the mussel *Mytilus galloprovincialis* to different reduced seawater salinities and its effect on several biochemical markers was probed and biotests were established. This investigation expands understanding of the multi-factorial effects of the physical marine environment on the specificity of investigated biomarkers and biotests, providing insight into the acclimation, adaptive and stress-response processes of mussels (Hamer et al., 2008).

Application of the European Union Water Framework Directive

A new method for the application of the European Union Water Framework Directive in the northern Adriatic has been developed. Extensive coastal investigations were carried out to map macroalgae distribution in the northern Adriatic and to relate their growth characteristics with anthropogenic influence and water quality levels (Iveša et al., 2008).

Monitoring the health status of patients

Current research, in collaboration with medical personnel from a local hospital, using surface-confined and bulk powder X-ray diffraction has indicated that renal and urinary biomineralized calculi might not grow evenly or have a uniform distribution of constituents. This suggests the preferential

inclusion of dominant compounds in the local environment in vivo, and the temporal variance of the dominance of those different compounds may be indicative of the health status of the individual (Lyons et al., 2008).



Figure 5. External morphology of a large human calculus showing non-homogeneous crystal growth and composition.

Mosquitofish as a bioindicator for pesticide pollution

The mosquitofish *Gambusia affinis*, due to its biological-ecological characteristics and due to the biomarker dose-response (MFO and DNA integrity), is suitable for monitoring of freshwater organochlorine pesticide contamination in general and lindane in particular. The conclusions are based on laboratory experiments with model pesticides and analysis of fish living in five Istrian natural ponds with different pollution loads.

Analysis of the p63 gene in mollusc

Two partial cDNA sequences and one partial genomic sequence, all originating from two different p63 alleles were found in one *Mytilus galloprovincialis* individual. The exon/intron architecture, DNA and deduced protein sequences were analyzed and compared to p53, p63 and p73 sequences from other organisms. The analysis showed our cDNA sequences code for the TAp63 γ isoform of p63 protein and identified all other molluscan p53

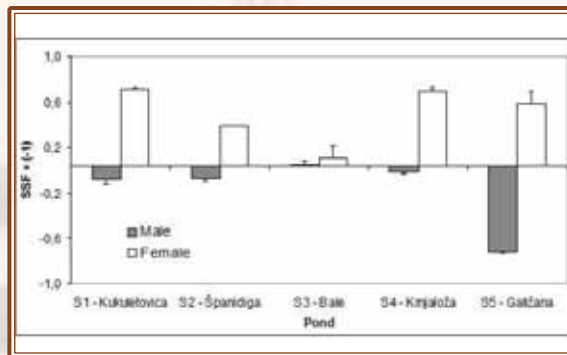


Figure 6. EROD activity in A) male and B) female *Gambusia affinis* liver homogenates from ponds, south-western Istrian peninsula. The results are given as a mean values with corresponding standard deviations. The levels of statistical significance (* $P < 0.01$ and $\square P < 0.05$) with a reference site sample (S3 - Bale pond) are indicated.

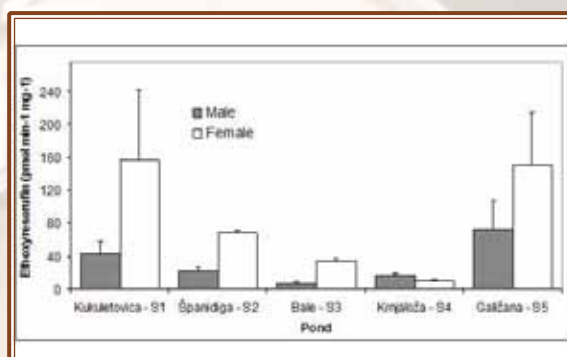


Figure 7. DNA integrity in A) male and B) female *Gambusia affinis* liver homogenates from ponds, south-western Istrian peninsula, Croatia. The results are given as a mean values with corresponding standard deviations. The levels of statistical significance (* $P < 0.01$) with a reference site sample (S3 - Bale pond) are indicated.

family sequences as p63 genes or their expression isoforms. Our results also indicate p63 as the ancestral gene of the p53 family as well as the only gene of the family present in pre-chordate metazoan species.

Marine pollutants and hypoosmotic conditions cause stress in the mussel *Mytilus galloprovincialis*

The level of acid DNase activity in the hemocytes and digestive gland of the mussel *Mytilus galloprovincialis* changed after exposure to detergent, gasoline and copper salt, as well as to unknown environmental mixture at selected sampling sites. Field investigations indicated that the digestive gland

is a suitable tissue for discrimination of polluted areas from mariculture areas. Seawater salinity variation (hypoosmotic stress) in the marine environment can affect all investigated parameters (DNA integrity, p38- MAPK activation, metallothionein induction, oxygen consumption rate and condition index).

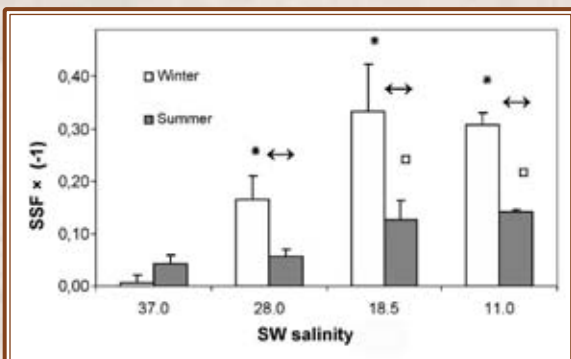


Figure 8. Negative DNA integrity $SSF \times (-1)$ values measured in gill homogenates of mussels acclimated to different SW salinities during high (summer) and low (winter) seawater temperatures. The results are presented in mean values of 4 or 5 gills (each derived from a single mussel) samples with the corresponding standard deviations. Statistically significant differences ($P < 0.05$) between mussels subjected to SW of 37 and lower salinities in the winter (*) and summer (↔), and between mussels acclimated to same salinity in winter and summer (↔) season are indicated.

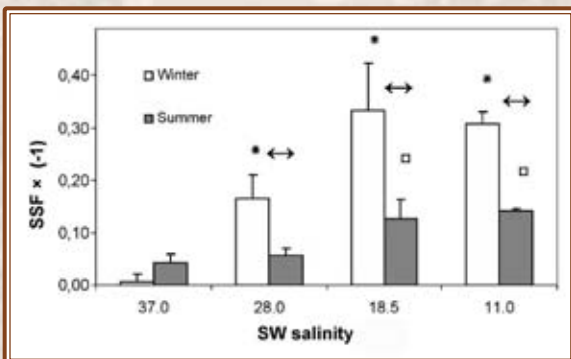


Figure 9. Similarity analysis of total mussel gills proteins after 1D SDS-PAGE separation: Lim mariculture, mussels subjected finally to 37, 28, 18.5, and 11 salinity during a 14-day acclimation in summer. Differently expressed proteins are indicated by dashed lines. A similarity analysis from the acclimation expression protein profiles was performed using an UDGMA algorithm.

Application of flow cytometry in marine environmental research

For the first time, the genome sizes of sea mouse and spiny crab were detected by

cell cycle and genome size analysis of five marine invertebrates with flow cytometry. Flow cytometry analysis was also introduced as fast and easy to the performed method for determination of micronuclei in mussels treated with model pollutants.

New equipment

Dcode system for Denaturing gradient gel electrophoresis (DGGE) is used for characterization of bacterial population structure and dynamics. The method can rapidly provide a characterization of community diversity and composition, and shifts in population can be readily demonstrated.

The Rigaku Ultima IV multipurpose X-ray, a fully-equipped state-of-the-art diffractometer, includes both parafocusing and parallel beam geometries, SAXS and WAXS abilities as well as micro area diffraction and accepts both solid and liquid-based samples. The new X-ray diffraction facilities have already attracted numerous external scientists to establish scientific collaborations.

EDUCATION

The Centre is involved in the organisation of Marine Sciences Studies (undergraduate) at the Juraj Dobrila University in Pula. This is the first time that university courses are performed at our department. The majority of courses are organized by Centre's scientists. Post-graduate courses were given at the Zagreb, Osijek and Dubrovnik universities.

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sport

1. Impact of pollution on programmed biosynthesis in marine invertebrates, Renato Batel
2. Ecotoxic effects of contamination on marine organisms, Nevenka Bihari
3. Biomineralization processes in marine organisms, Davorin Medaković

4. Structure and physiology of microbial communities in northern Adriatic fronts, Mirjana Najdek
5. Mechanism of long-term changes in the northern Adriatic ecosystem, Robert Precali
6. Biodiversity of benthic communities in the Adriatic: natural and human impacts, Ana Travizi

Programs supported by the Ministry of Sciences, Education and Sports

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

Research, developmental and international projects

1. Schwaemme aus Rovinj (Kroatien)-Extract-bereitstellung und Marikultur, Project: Molekulare Biotechnologie und Wirkstoffe mariner Schwaemme sowie Schwamm-assoziiierter Mikroorganismen, Renato Batel, Werner E.G. Müller (Croatian German scientific project)
2. Biocapital, Marie Curie Research Training Network, Renato Batel, Werner E.G. Müller (EU-FP6, 2005-2008)
3. Realization of an integrated monitoring system of the quality of the Adriatic Sea, with particular regard to eutrophication and mucilage phenomena (REQUISITE), Danilo Degobbis (EU INTERREG IIIA, 2004-2006, extension 2007-2008)
4. Integrated system for monitoring and forecasting of meteorological and water conditions parameters in the Adriatic Sea (ADRIAMET), Danilo Degobbis (EU INTERREG IIIA, 2004-2008)
5. Anossie attuali nel nord Adriatico, registrazione nei sedimenti in epoca storica, influenza sulle risorse di pesca e bentoniche. Modellizzazione e previsione (ANOCISA), Robert Precali (Ministero dell'Istruzione, dell'Università e della Ricerca della Repubblica Italiana, 2004-2008)
6. Monitoring of the marine coastal current of the north Adriatic (NASCUM), Nenad Smolaka (2007-2008)

7. Implementation of the water quality monitoring in the western Istrian coastal sea (northern Adriatic) (WICOS), Tamara Đakovac (INTERREG-CARDS/PHARE 2008-2009)
8. Proteomique des Mollusques et Biomineralisation, ProMoBio, F. Marin, D. Kotrošan, Davor Medaković (Egide ECO-NET, France, 2008-2010)
9. Carboanhydrase - Gehalt / Aktivität und Biomineralisation in Mittelmeermuscheln und Schwämmen, Hans C. Schröder, Bojan Hammer (Internationales Büro des Bundesministerium für Bildung und Forschung – BMBF, MOE 08/R55, 2008-2009)
10. Development of a Sensor for Marine Biotoxins, Daniel M. Lyons (Royal Society of Chemistry UK, SensBioTox IRG-4-2008)

SELECTED INVITED LECTURES

1. Devescovi M. Impatto delle mucillagini sul macrobentos della costa istriana. Corso di Studio in Scienze Ambientali Marine ed Oceanografia, org. Università di Bologna in Ravenna, Rovinj, 18 June 2008.
2. Jaklin A. North Adriatic macrobenthos, Corso di Studio in Scienze Ambientali Marine ed Oceanografia, org. Università di Bologna in Ravenna, Rovinj, 18 June 2008.
3. Travizi A. Meiofauna as a tool for environmental quality assessment, Corso di Studio in Scienze Ambientali Marine ed Oceanografia, org. Università di Bologna in Ravenna, Rovinj, 19 June 2008.
4. Iveša Lj, Devescovi M. Assessment of the ecological status of north-eastern Adriatic coastal waters (Istria, Croatia) using macroalgal assemblages for the European Union Water Framework Directive, Workshop Biological Assessment, Coastal waters, European Union Twinning Project Implementing of the Water Framework Directive in Croatia "Biological assessment of transitional and Coastal waters", workshop, Trogir, 30 June 2008.
5. Travizi A. Implementing the Water Framework Directive in Croatia: Macroinvertebrates, Croatian approach, European Union Twinning Project Implementing of the Water Framework Directive in Croatia "Biological assessment of transitional and Coastal waters", workshop, Trogir, 30 June 2008.
6. Mičić M, Gobić Medica K, Medica M, Lazar B. Flow cytometric analysis of loggerhead

turtle (*Caretta caretta*) peripheral blood cells from north Adriatic Sea, Third Mediterranean Conference on Marine Turtles, Yasmine Hammamet, Tunisia, 20-23 October 2008.

7. Medaković D. X-ray diffraction methods in biological, ecological and medical research, Međunarodni Forum Bosna, Centar za prirodno naslijeđe, Sarajevo, Bosnia and Herzegovina, 18 November 2008.
8. Medaković D. Apoxyomenos, Application of X-ray diffraction and spectroscopic methods in archaeology and museology, Zemaljski muzej Bosne i Hercegovine, Sarajevo, Bosnia and Herzegovina, 20 November 2008.

SELECTED ORGANIZED CONFERENCES

1. School of Conservation Biology of the Croatian Biological Society in affiliation with Ruđer Bošković Institute, Centre for Marine Research, Rovinj, 20-28 June 2008. Hamer B (Vice Chair), Smolaka N (Financial director), Pavičić-Hamer D (Organizing committee).

SELECTED PUBLICATIONS

Review articles

1. Marin F, Luquet G, Marie B, Medakovic D. Molluscan Shell Proteins: Primary Structure, Origin, and Evolution. In: Current Topics in Developmental Biology, Schatten, P Gerald (ed.). Pittsburgh: Elsevier Science & Technology Books, 2008, pp. 209-276.

Scientific papers

1. Fafandjel M, Bihari N, Perić L, Cenov A. Effect of marine pollutants on the acid DNase activity in the hemocytes and digestive gland of the mussel *Mytilus galloprovincialis*. Aquatic Toxicology 2008: 86: 508.

2. Fafandjel M, Bihari N, Smolaka M, Ravlić S. Hemocytes/ coelomocytes DNA content in five marine invertebrates: cell cycles and genome sizes. Biologia 2008: 63: 730.
3. Hamer B, Jakšić Ž, Pavičić-Hamer D, Perić L, Medaković D, Ivanković D, Pavičić J, Zilberberg C, Schröder HC, Müller WEG, Smolaka N, Batel R. Effect of hypoosmotic stress by low salinity acclimation of Mediterranean mussel *Mytilus galloprovincialis* on biological parameters used for pollution assessment. Aquatic toxicology 2008: 89: 137.
4. Iveša L, Lyons DM, Devescovi M. Assessment of the ecological status of northeastern Adriatic coastal waters (Istria, Croatia) using macroalgal assemblages for the European Union Water Framework Directive. Aquat. Conserv. 2008: DOI: 10.1002/aqc.964.
5. Jakšić Ž, Hamer B, Landeka N, Batel R. Western mosquitofish as a bioindicator of exposure to organochlorine compounds. Ecotoxicology & Environmental Safety 2008: 71(2): 426.
6. Lucu Č, Pavičić J, Ivanković D, Pavičić-Hamer D, Najdek M. Changes in Na⁺/K⁺-ATPase activity, unsaturated fatty acids and metallothioneins in gills of the shore crab *Carcinus aestuarii* after dilute seawater acclimation. Comparative Biochemistry and Physiology 2008: 149A: 4: 362.
7. Marie B, Luquet G, Bédouet L, Milet C, Guichard N, Medaković D, Marin F. Nacre calcification in the freshwater mussel *Unio pictorum*: carbonic anhydrase activity and purification of a 95-kDa calcium-binding glycoprotein. ChemBioChem 2008: 9 (15): 2515.
8. Vilibić I, Beg Paklar G, Žagar N, Mihanović H, Supić N, Žagar M, Domijan N, Pasarić M. Summer breakout of trapped bottom dense water from the northern Adriatic. Journal of Geophysical Research - Oceans 2008: 113: S1102-1.
9. Zucht, W., Sidri, M., Brümer, F., Jaklin, A., Hamer, B. Ecology and distribution of the sponge *Aplysina aerophoba* (Porifera, Demospongiae) in the Limski kanal (Northern Adriatic Sea, Croatia). Fresenius Environmental Bulletin 2008: 17(7): 890.

ORGANISATION OF THE CENTRE

Head: Karolj Skala

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

- ⇒ Laboratory for Optoelectronics and Visualisation, Karolj Skala
- ⇒ ICST research and development, Davor Davidović
- ⇒ Information systems, Nikola Pavković
- ⇒ Service and maintenance, Đuro Kuzumilović



the integration of user interfaces and interactive work in virtual and real space, including human-machine interaction.

On top of a national scientific program and various domestic projects, CIR has a very healthy international presence. For example, CIR participates in contracted collaborative work with 125 EU institutions based on the EU FP 6 and FP7 framework programmes. The Centre is a member of the Networked European Software and Services Initiative (NESSI), which is a European Technology Platform for Software and Services. In addition, CIR has substantial collaborative interactions with CERN (Geneva, Switzerland), Jožef Štefan Institute (Ljubljana, Slovenia), Technical University Budapest (Budapest, Hungary), and the Institute for Parallel Processing (Sofija, Bulgaria).

OVERVIEW OF THE CENTRE

Scientific Research and Development

In addition to being responsible for the coordination and maintenance of the informatics and computing infrastructure at the RBI, CIR is also actively engaged in a scientific and research programme. The mission of this programme is the advancement of computer usage in scientific work, based on development of the e-science technologies as the next generation of knowledge infrastructure to support computationally based science.

The R&D group has experience in signal processing, computer graphics, parallel algorithms, visual interfaces, visual peripherals,

TOP ACHIEVEMENTS OR HIGHLIGHTS IN 2007

Enabling Grids for E-science (EGEE)

The CRO-GRID JRU (Joint Research Unit), finished the work in the EU FP6 EGEE-II project and started with EGEE III through-

out 2008. In addition to the existing PARF (Parallel Random Forests classification) and QRBGS (Quantum Random Bit Generator Service), <http://random.irb.hr/> a new service was introduced: the Protein Database Visualisation Generator (PDVG).

South Eastern European GRid-enabled e-Infrastructure Development (SEE-GRID)

In the EU FP6 SEE-GRID-2 project, as the leader of the Work Package (WP4), CIR actively worked on the collection and systematisation of gained knowledge on Applications Gridification, acting as the editor of a Deliverable to the EC.

Centre for Scientific Visualization (CenVis)

The accomplished goals of the CenVis EU FP 6 project during this year progress are seen in several large points such as infrastructure development, dissemination actions and regional and national cooperation. We upgraded existing e-Infrastructure with new processor cluster installation, the establishment of a visualization laboratory, selection, evaluation and acquisition of distributed computing and visualization equipment. The CenVis Informational portal (Vision point) up and running, promotional packages that include Grid and Visualization conference introduced on 31st International Convention MIPRO for the purpose of presenting the growing development of techniques and technologies in science.

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

Digital Research Infrastructure for the Arts and Humanities (DARIAH)

In the last quarter of 2008, the FP7 project DARIAH began. The initial efforts were mainly focused on building a sustainable web page. The new web page was built on a completely new system and new functionalities were added. We have been testing existing technologies focused on work with SRM protocol and GFAL libraries.



Figure 1. ICT 2008 Conference in Lyon, ATOMARIUM announced on 3D Display from Holografika and won second prize in "Best Exhibit" Award.

Information Systems development and service usage

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

Besides maintaining the core infrastructure ICT facilities and services, the Information systems department established a new infrastructure service – OpenVPN, which had entered the testing phase by the end of 2008. We also continued the effort to migrate all workstations to the internal network, providing better security for the end-user and the ICT system as a whole. Figure 2 shows

the per-month distribution of migrated workstations:



Figure 2. Number of workstation migrated to internal networks.

The main web-server (www.irb.hr), which provides information to the general public, is also maintained by the Information systems department. The CMS-driven core engine enables users to develop extended functionality web-applications such as time-schedule applications etc. Figure 3 shows the per-month distribution of unique visits:

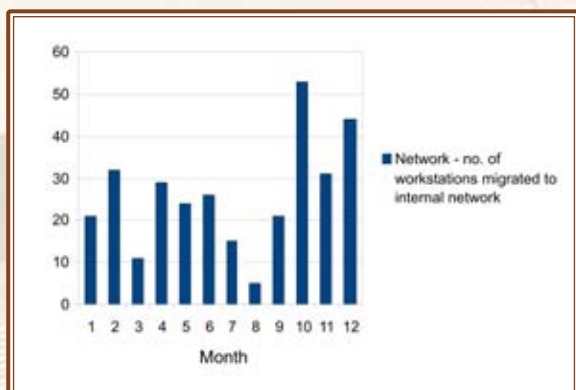


Figure 3. Number of visitors to the RBI web domain.

User support

Our helpdesk is continuing its usage of OTRS ticketing system, which has proven itself to be an indispensable tool for everyday operations. Figure 4 shows the per-month distribution of resolved issues tracked by OTRS.

Printing and teleconferencing services continued to function without any major problems. Figure 5 shows the statistics of the public printing service.

The number of user accounts is slightly increasing, with Figure 6 showing the number of new user accounts added each month.



Figure 4. Number of resolved tickets.



Figure 5. Number of printed pages.

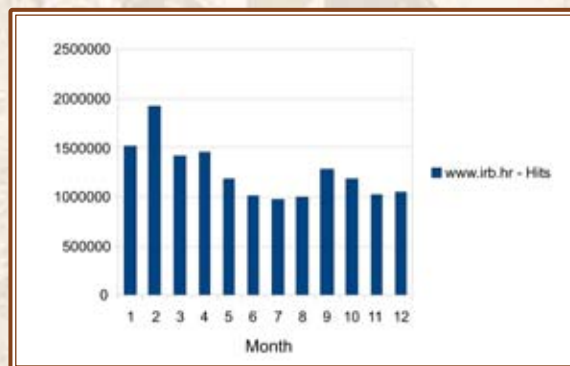


Figure 6. Number of LDAP user accounts.

Project initiatives

CIR prepared seven EU FP7 project proposals for ICT Calls in 2008. In this way, we aim to continue the e-Science program ori-

entation and form a project chain on the line of e-Infrastructure, distributed computing, parallel applications and scientific visualisation technologies. We also started with Atomarium project initiatives. This project consists of distributed network storage of micro world (atoms, genes, proteins etc.) of virtual images that comes from daily rendering on a Grid infrastructure and provides search and 2/3D display in the Atomarium in much the same way as planetarium displays planets (macro world). At the ICT 2008 Conference in Lyon, ATOMARIUM announced on 3D Display from Holografika and won second prize in "Best Exhibit" Award.

New Equipment

Inside the framework of the Croatian National Grid Infrastructure CRO NGI a new HP blade 96 processor cluster was installed at RBI, for furthering scientific research. During 2008 CIR continued the eScience programme based on ICST (Information Communication Science Technology) on Grid platforms. The Scientific Visualization Laboratory was completed. A number of active network devices were acquired and deployed with aim of extending network capacity of the RBI core network. These consist of mainly Cisco GB switches.

EDUCATIONAL ACTIVITIES

CIR provides 5 undergraduate and 3 graduate courses at Faculty of Electrical Engineering and computing and Faculty of Graphical Arts at the University of Zagreb. We also hosted the High Performance Computing on Grid for Meteorological Applications Workshop, encompassing present cluster and grid technologies and the WRF prognostic model to wider public with special focus on the meteorological community. As part of FP project initiatives, courses and seminars were held in cooperation with several universities in Zagreb. For the benefit of training, an experienced researcher was

brought in from a European Institute for the purpose of lecturing.

ORGANISATION OF CONFERENCES AND SPORTING EVENTS

CIR organized the annual Conference Grid and Visualisation Systems as part of the International Convention MIPRO in Opatija (<http://www.mipro.hr/gvs.htm>).

PROJECTS AND PROGRAMS

Projects supported by Ministry of Sciences, Education and Sports

1. Scientific Visualisation Methods, Karolj Skala

Programs supported by the Ministry of Sciences, Education and Sports

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

International EU FP6 projects

1. Grid enabled Infrastructure Development, SEE GRID, EU F6, 002356, Karolj Skala
2. Enabling Grids for E-science-II (EGEE-II), EU F6, 031688, Karolj Skala
3. South Eastern European GRid-enabled eInfrastructure Development 2 (SEE GRID 2) EU FP6, 031775, Karolj Skala
4. Centre for Scientific Visualisation (CenVis), EU FP6, 043947, Karolj Skala
5. Interactive Visual Analysis of Bio-signals – IVAB, SEE ERA NET, Karolj Skala

International EU FP7 projects

1. Enabling Grids for E-science-III (EGEE-III), EU FP7, Con. no. 222667, Karolj Skala
2. South Eastern European GRid-enabled eInfrastructure Development 2 (SEE GRID SCI) EU FP7, Con. no. 211338, Karolj Skala
3. Digital Research Infrastructure for the Arts and Humanities, DARIAH Con. no. 211583, Karolj Skala

SELECTED PUBLICATIONS

1. Karainova A, Atanassov E, Gurov T, Stevanovic R, Skala K: Variance Reduction MCMs with Application in Environmental Studies: Sensitivity Analysis. Applications of Mathematics in Engineering and Economics. New York: American Institute of Physics, 2008. pp. 549-558.
2. Kolarić D, Skala K, Dubravić A: Integrated System for Forest Fire Early Detection and Management, Period Biol 2008: 110: 205.



ORGANIZATION OF THE CENTRE

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

The Centre consists of the following laboratories:

- ⇒ Laboratory for NMR spectroscopy and modelling, Dejan Plavšić
- ⇒ Laboratory for glasses, Andrea Moguš-Milanković



OVERVIEW OF THE CENTRE

The Centre for NMR conducts scientific research and performs services for scientists and researchers from the academic community, governmental institutions and industry in Croatia. The basic equipment of the Centre consists of Bruker Avance 300 and 600 MHz NMR spectrometers and a Varian Gemini 300 MHz NMR spectrometer located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb.

In 2008, the members of the Centre made valuable contributions to peptide and organometallic chemistry, photochemistry, biochemistry, chemical graph theory, and solid state chemistry. These contributions were published in high ranking journals and a patent was taken out. The scientists of the Centre continued to be involved in lecturing at the Universities of Zagreb, Split, Osijek, and Rijeka and organized a number of scientific

conferences and courses. Active collaborations with research groups in USA, Austria, Slovenia, Germany, Romania, Hungary, Turkey, Brazil, Russia, and the Czech Republic were maintained.

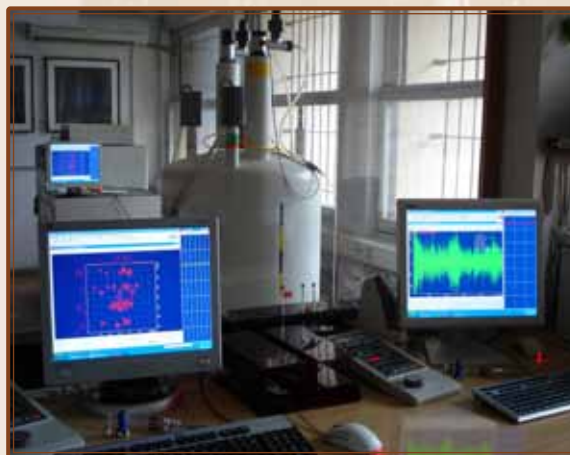


Figure 1. The NMR operators' room with a view on a 7T magnet.

TOP ACHIEVEMENTS

Assignment of NMR spectra of new compounds

Novel β -3-thienyl and β -3-furyl derivatives of o-divinylbenzene have been synthesized and their photochemical behaviour compared with 2-thienyl and 2-furyl derivatives. Photochemical reactions were monitored and products were determined by NMR spectroscopy (Vidaković et al., 2008).

Cadmium(II) complexes of 3-hydroxypicolinic acid, $[\text{Cd}(\text{3-OHpic})(\text{3-OHpicH})(\text{H}_2\text{O})_2]$, $[\text{Cd}(\text{3-OHpic})_2(\text{H}_2\text{O})_2]$, and $[\text{Cd}(\text{3-OHpic})_2]_n$, were prepared and characterized by NMR spectroscopy. In the DMF solution of all the prepared complexes, only the monodentate mode of 3-OHpicH binding to cadmium(II) through the carboxylate O atom was determined by ^1H , ^{13}C , ^{15}N and ^{113}Cd NMR spectroscopy (Kukovec et al., 2008).

A number of derivatives of thymol, carvacrol, and eugenol were synthesized and their structures determined by NMR spectroscopy. The obtained derivatives showed remarkably better antioxidative properties according to 1,1-diphenyl-2-picrylhydrazyl and Rancimat assays in comparison with parent compounds and similar antioxidative properties to butylated hydroxytoluene and vitamin C (Mastelić et al., 2008).

Application of methods of discrete mathematics to various chemical problems

It has been shown that topological considerations based on the eigenvectors of the Laplacian matrix are able to give reasonable shapes of pure carbon nanotube junctions (Graovac et al., 2008).

The well known Zagreb and variable Zagreb indices M1 and M2 have been studied and in the case of acyclic molecules unexpected inequalities among these indices have been proven (Vukičević and Graovac, 2008).

Correlation between microstructure and electrical properties of ZrTiO_4 ceramics

A series of ZrTiO_4 ceramics were prepared by sintering ball-milled precursor powders. Ceramics with homogeneously dispersed micropores containing both low-temperature (ordered) and high-temperature (disordered) ZrTiO_4 phases were achieved by sintering at 1400°C . The porosity and the morphology were modified by changing the sintering time. The impedance spectra followed the observed changes in the ceramics' microstructure. The grain boundaries' shape, rather than the grain size, has the major influence on the conductivity. The lowest value for electrical conductivity, $8.1 \times 10^{-10} (\Omega \cdot \text{m})^{-1}$, was obtained in the ceramics sintered at 1400°C for 4 h. This confirms the blocking effect of the imperfect grain boundaries; i.e., the defects of the grain boundaries, which were formed during the grain growth, were followed by an almost complete loss of pores (Ličina et al., 2008).

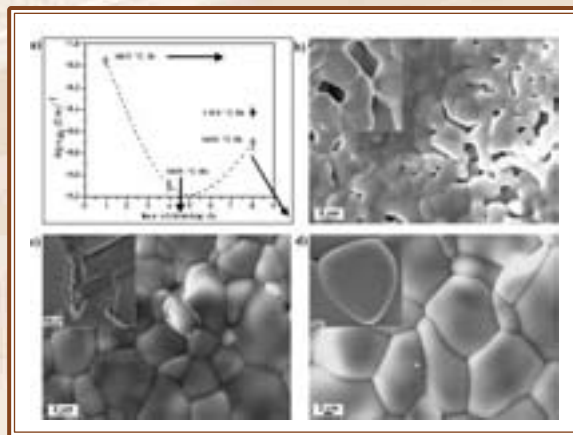


Figure 2. a) Changes of the DC conductivity for ZrTiO_4 ceramics sintered at various temperatures and times, b) SEM images of samples sintered at 1400°C for 1 h, c) 4 h, d) and 8 h. The insets show HRSEM images.

Patent

PCT/HR2008/000037, 11989. Kopriva I, Jerić I, Smrečki V. Method of and system for

blind extraction of more than two pure components out of spectroscopic or spectrometric measurements of only two mixtures by means of sparse component analysis.

EDUCATION

In 2008, the members of the Centre taught 5 undergraduate and 9 postgraduate courses at Universities in Zagreb, Split, Osijek, and Rijeka.

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sports

1. NMR Spectroscopy and Modelling of Bioactive Molecules, Dejan Plavšić
2. Modelling of molecules and materials by methods of mathematical and computational chemistry, Ante Graovac.
3. Modelling of bioactive molecules and testing of their properties and activity, Nikola Štambuk
4. Influence of structure on electrical properties of (bioactive) glasses and ceramic, Andrea Moguš-Milanković

Research, developmental and international projects

1. Multi-field experimental high resolution NMR studies with applications to bioactive compounds, Vilko Smrečki, (MSES, bilateral collaboration with Austria, WTZ HR 19/2008)
2. Applications of topological, geometric, algebraic and combinatorial methods in sciences, Ante Graovac (MSES, bilateral collaboration with Slovenia).
3. Investigation of the ion dynamics in ionic liquids by measuring their frequency-dependent mechanical properties, Ana Šantić (Postdoctoral project, NFS Croatia, Institute of Physical Chemistry, University of Münster, Germany)
4. Novel method to support bone growth bioactive glass coated with protein/lipid poroxidation products, Nationalbank Jubiläumsfonds Grant (Nr. 12611), LKH Graz, Renate Wild-

burger (Neven Žarković, Andrea Moguš-Milanković)

5. The origin of structural defects and their influence on macroscopic properties of solar silica glass, Davor Gracin (Andrea Moguš-Milanković), (NFS Croatia, Ruđer Bošković Institute-Lipik Glas d.o.o.)

Contracts with industry

1. Collaboration contract with PLIVA d.d.
2. Collaboration contract with BELUPO d.d.
3. Collaboration contract with Croatian Institute of Viticulture and Enology
4. Collaboration contract with Lipik Glass d.o.o.

SELECTED INVITED LECTURES

1. Graovac A. Topological coordinates for carbon nanotubes junctions. The First Conference and Workshop on Mathematical Chemistry, Tarbiat Modares University, Teheran, Iran, January 29-31, 2008.
2. Graovac A. On two rather different applications of directed graphs to chemistry. Workshop on Metric Graph Theory and Applications, Isfahan Institute of Technology, Isfahan, Iran, February 2-3, 2008.
3. Graovac A, Laszlo I, Pisanski T. Shape analysis of carbon nanotubes junctions. The 23rd International Conference MATH/CHEM/COMP 2008, Verbania, Italy, June 10-13, 2008.
4. Šantić A. Ion dynamics in room temperature ionic liquids - II, complex fluidity measurements. Institute of Physical Chemistry, University of Münster, Germany, June 19, 2008.
5. Štambuk N. Molecular recognition theory and its application in vaccine development and toxicology. BIT Life Sciences 1st World Congress of Vaccine, WCV-2008, Foshan, China, December 1-5, 2008.

SELECTED ORGANIZED CONFERENCES AND COURSES

1. Regional Training Course on How to Write Competitive Research Proposals for Various Funding Programmes, RER/0/023, IAEA, Zagreb, Croatia, March 18–20, 2008, organized by A. Moguš-Milanković.

2. The 23rd International Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Verbania, Italy, June 10-13, 2008., organized by A. Graovac.
3. The 23rd International Course on the Interfaces among Mathematics, Chemistry and Computer Sciences, Dubrovnik, Croatia, June 16-21, 2008., organized by A. Graovac, D. Vikić-Topić, D. Plavšić.
4. The 10th Central European NMR Symposium & The 10th Central European Bruker NMR Users Meeting, Zagreb, Croatia, September 29-30, 2008, organized by V. Smrečki.

SELECTED PUBLICATIONS

1. Vidaković D, Škorić I, Horvat M, Marinić Ž, Šindler-Kulyk M. Photobehaviour of 2- and 3-heteroaryl substituted o-divinylbenzenes; formation of fused 2,3- and 3,2-heteroarene-benzobicyclo[3.2.1]octadienes and 3-heteroaryl enzobicyclo[2.1.1]hexenes. *Tetrahedron* 2008: 64: 3928.
2. Kukovec BM, Popović Z, Pavlović G, Vinković M, Vikić-Topić D. Synthesis and characterization of some novel cadmium(II) complexes with 3-hydroxypicolinic acid (3-OHpicH). Crystal and molecular structures of $[\text{Cd}(\text{3-OHpic})(\text{3-OHpicH})(\text{H}_2\text{O})]_2$, $[\text{Cd}(\text{3-OHpic})_2(\text{H}_2\text{O})_2]$ and $[\text{Cd}(\text{3-OHpic})_2]_n$. *Polyhedron* 2008: 27: 1479.
3. Mastelić J, Jerković I, Blažević I, Poljak-Blaži M, Borović S, Ivančić-Baće I, Smrečki V, Žarković N, Brčić-Kostić K, Vikić-Topić D, Müller N. A comparative study on the antioxidant and biological activities of carvacrol, thymol and eugenol derivatives. *J Agr Food Chem* 2008: 56: 3989.
4. Graovac A, Laszlo I, Pisanski T. Shape analysis of carbon nanotube junctions. *MATCH-Commun Math Comput Chem* 2008: 60: 917.
5. Vukičević D, Graovac A. Comparing variable Zagreb M1 and M2 indices for acyclic molecules. *MATCH-Commun Math Comput Chem* 2008: 60: 37.
6. Ličina V, Gajović A, Moguš-Milanković A, Djerdj I, Tomašić N, Su DS. Correlation between the microstructure and the electrical properties of ZrTiO_4 ceramics. *J Am Ceram Soc* 2008: 91: 178.

Head of Library: Jadranka Stojanovski



OVERVIEW OF LIBRARY ACTIVITIES

The information landscape of early twenty-first century research is characterized by easy and simple online access to the digitized content. Researchers are beginning and ending their quest for information online. In this sense, we are constantly rethinking the RBI Library as a part of the dynamic and changing landscape dominated by digital technology. Changes of the research and scholarly communication in general should be followed by the development of library services and continuous redefinition of library functions. This includes strong collaboration between librarians, researchers, and information technology experts to articulate strategies and tactical approaches to a rapidly changing environment.

GOALS AND OBJECTIVES

In 2008 our virtual entity was recognized well by library users and the average number of visits of our library web site was more than 3500 daily and constantly growing. The present state of Library web site is not getting the best from newest technologies, and library web site complete redesign becomes a priority.

The development of institutional repositories emerged as a new strategy that allows research institutes and universities to apply systematic leverage to accelerate changes taking place in scholarship and scholarly communication, both moving beyond their relatively passive role of supporting big commercial publishers in modernizing scholarly publishing through the licensing of digital content. Many technology trends and development efforts came together to make this strategy possible. Supporting software programmes are well developed and free of charge, online storage costs have dropped significantly and repositories are now affordable. Standards like the open archives metadata harvesting protocol (OAI-MHP) are widely accepted.



Figure 1. Library web site.

The thinking about digital preservation over the past five years has advanced to the point where the needs are widely recognized and well defined. At RBI Library we started with digitization of photographic materials in 2008. All digital materials are stored in the institutional repository based on ePrints.

In 2008 RBI Library focused the efforts in building a comprehensive bibliography of RBI papers, together with their citations from Web of Science database. It is well known that scholarly writing is grounded in prior research. Citations are demonstrating that RBI publications are referenced and addressed by authorities in the field. Bibliography will provide different bibliometric and scientometric analysis necessary for evaluation purposes to improve quality of the research.

COLLECTIONS

Digital collection

The journal acquisition model in 2008 continued to be realized through “big deals” with main world publishers as Elsevier, Springer, Blackwell, Nature Publ. etc., subscribed at the national consortia level directly by the Ministry of Sciences, Education and Sports (MSES). Beside 20.000 e-journals available to the Croatian academic community, RBI subscribed 57 e-journals of the smaller, but not less important publishers. The access to the e-journal collection, as to the relevant bibliographic and full-text databases, was realised mainly through the Centre for online databases (<http://www.online-baze.hr>) and in-house developed RBI Library portal to e-journals Pero (<http://knjiznica.irb.hr/pero>), which became very popular inside the research community. Over 60 fee and free databases, over 20.000 e-journals and 42 e-books were available to RBI researchers.

Printed collection

While the organization and accessibility of digital resources accounted for most of our

time and attention, even the reduced numbers of print publications remained an important part of our collection and will continue to do so well into the future. In 2008, we subscribed 90 printed journals as addition to the electronic version. Lack of stable financing and delays in subscription, supported by publisher’s subscription policies not guaranteeing continuous access, made subscribed digital content fragile and unreliable. The book collection amounts to 22,173 volumes, 491 of which were newly acquired in 2008.



Figure 2. Library during Open days.

Interlibrary loan

The RBI Library collection, which represents accumulated knowledge, besides being a tool that makes research and scholarship possible at RBI, serves scholarly community in Croatia and abroad. The RBI Library has a well-established interlibrary loan service with other libraries mainly from Croatia, Germany, United Kingdom and USA. In 2008, it fulfilled 870 requests for documents made by RBI staff, and over 495 requests from other libraries. Interlibrary loan requests have been handled through online application SEND developed in-house. Through cooperation with numerous libraries we have built and extensive shared collection of greater depth than any of the libraries could build alone.

SERVICES

The RBI Library web site is the place where we offer our digital collections and services. The Library web site is the main access point to the online catalogue and networked resources, carefully selected and organized. In 2008, the Library web site received over 100,000 visits in an average month. The virtual library serves the same diverse population as the physical library, so we organize it to accommodate multiple levels of researcher's demands. The Library web site is created and maintained by Library staff for the benefit of the entire research community.

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

- Library Colloquia (<http://knjiznica.irb.hr/hrv/kolokviji.html>)
- Library Blog (<http://knjiznica.irb.hr/blog>)
- PERO – e-journals portal (<http://knjiznica.irb.hr/pero>)
- SEND - Interlibrary Loan service (<http://send.irb.hr>)
- CROSBİ – Croatian Scientific Bibliography (<http://crosbi.znanstvenici.hr>)
- Who's Who in Croatian Science (<http://tkojetko.znanstvenici.hr>)
- HRČAK – portal of Croatian scientific journals (<http://hrcak.znanstvenici.hr>)
- CMS for web sites of Croatian academic and research libraries (<http://knjiznice.szi.hr>)
- Centre for online databases (<http://www.online-baze.hr>).



Figure 3. Library Colloquia.

NEW LIBRARY MANAGEMENT SYSTEM

The new Library Management System, which was evaluated and selected by Croatian National and University Library for all Croatian higher education and research li-

braries, was still not implemented in libraries during 2008. The Voyager system was elected to support library functions such as acquisition, cataloguing, and interlibrary loan and financed by MSES for all Croatian academic and research libraries. Implementation of Voyager would permit the RBI Library to utilize state-of-the art technology for delivering services. As Voyager was not implemented, a decision was made for migration to the integrated library system KOHA, which is an open source software available to every library and supporting all modules. During 2008, the conversion from UNIMARC to MARC21 standard has been done as customisation of KOHA modules.

EDUCATION

Library staff members are involved in graduate level teaching at University J. J. Strossmayer in Osijek and University of Zadar.

As part of the Centre for continuing education of librarians we provide several Building digital collection courses.



Figure 4. Students (primary school) education.

CONFERENCE ORGANIZATION

The 8th Annual conference of the Croatian Academic and Scientific Libraries 2008 entitled "Scientific information management" was organized by the RBI Library, Croatian Academic and Research Network CARNet, the

Faculty of Philosophy, the Faculty of Economics and the Faculty of Civil Engineering, from 24-25 October 2008, with 200 participants.



Figure 5. Librarian's 2008 conference with information management as a main topic.

IT PROJECTS

In 2008, we continue our activities on the projects included in the Croatian Scientific Portal: Croatian Scientific Bibliography, Who's Who in Science in Croatia, HRČAK – portal of Croatian scientific journals, Pair of Compasses – inventory of the scientific equipment although without the formal contract with MSES and proper financing. The project Centre for online databases was realized through cooperation with the Croatian Academic and Research Network (CARNet) and MSES.

SELECTED LECTURES

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2. Stojanovski J. International visibility of the Croatian scientific output and HRČAK role (in Croatian). CUC 2008: Internet 10.0. Rijeka, Croatia, 10-12 November 2008.
3. Stojanovski J. Science in Croatia. TEMPUS "Capacity Building for Research in Croatia", Zadar, Croatia, October 30, 2008.

SELECTED PUBLICATIONS

1. Konjević S. Chemical Education Digital Library. Chemistry in industry 2008: 57: 323.
2. Macan B. Detronization of impact factor?! - appearance of the new, free benchmark SCImago Journal Rank (in Croatian). Chemistry in industry 2008: 57: 262.
3. Macan B, Stojanovski J. Analysis of the Ministry of Sciences, education and sports financial support of Croatian scientific journals (in Croatian). Chemistry in industry. 2008: 57: 115.
4. Mayer M. Depth-First: Walking the Web of Chemical Information. Chemistry in industry 2008: 57: 70.
5. Mayer M. Interlibrary loan - what, why, how and how much (in Croatian)? Chemistry in industry 2008: 57: 380.



Rudjer Innovations Ltd.

<http://www.r-i.hr>

COMPANY ORGANIZATION

Head of Management Board, CEO:
Domagoj Oreb

Member of Management Board, CFO:
Dinko Smolčić

Member of Management Board:
Božidar Etlinger

Business Development Manager:
Davorka Moslavac Forjan

Business Development Manager:
Davor Aničić

Business Development Manager:
Lidija Stopfer

Project Analyst: Matea Novosel



OVERVIEW OF THE COMPANY

Rudjer Innovations (R-I) is a company specialised in commercialisation of innovations and technology transfer. It links science and technology with economy and industry.

The company is open both to the scientific community, including researchers and innovators, helping them commercialise innovations and scientific research results, and to companies that are willing to apply the know-how of the scientific community in their business operations.

Rudjer Innovations Ltd was founded with the full support of the Government and the World Bank as a daughter company of the Ruđer Bošković Institute (RBI). Its aim is to promote the cooperation and partnership of research institutes, universities and innovator communities with commercial entities.

Rudjer Innovations is open to the entire Croatian public.

The mission of R-I is to contribute to the development of Croatia as a knowledge society by linking the scientific and research community with enterprises and businesses and thus through commercialisation of knowledge strengthen the competitiveness of Croatia in the global market.

The goal is to establish a cooperation which brings mutual interest, ensuring a win-win result, with numerous competitive advantages for both companies and scientists.

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

TOP ACHEIVEMENTS

Portfolio

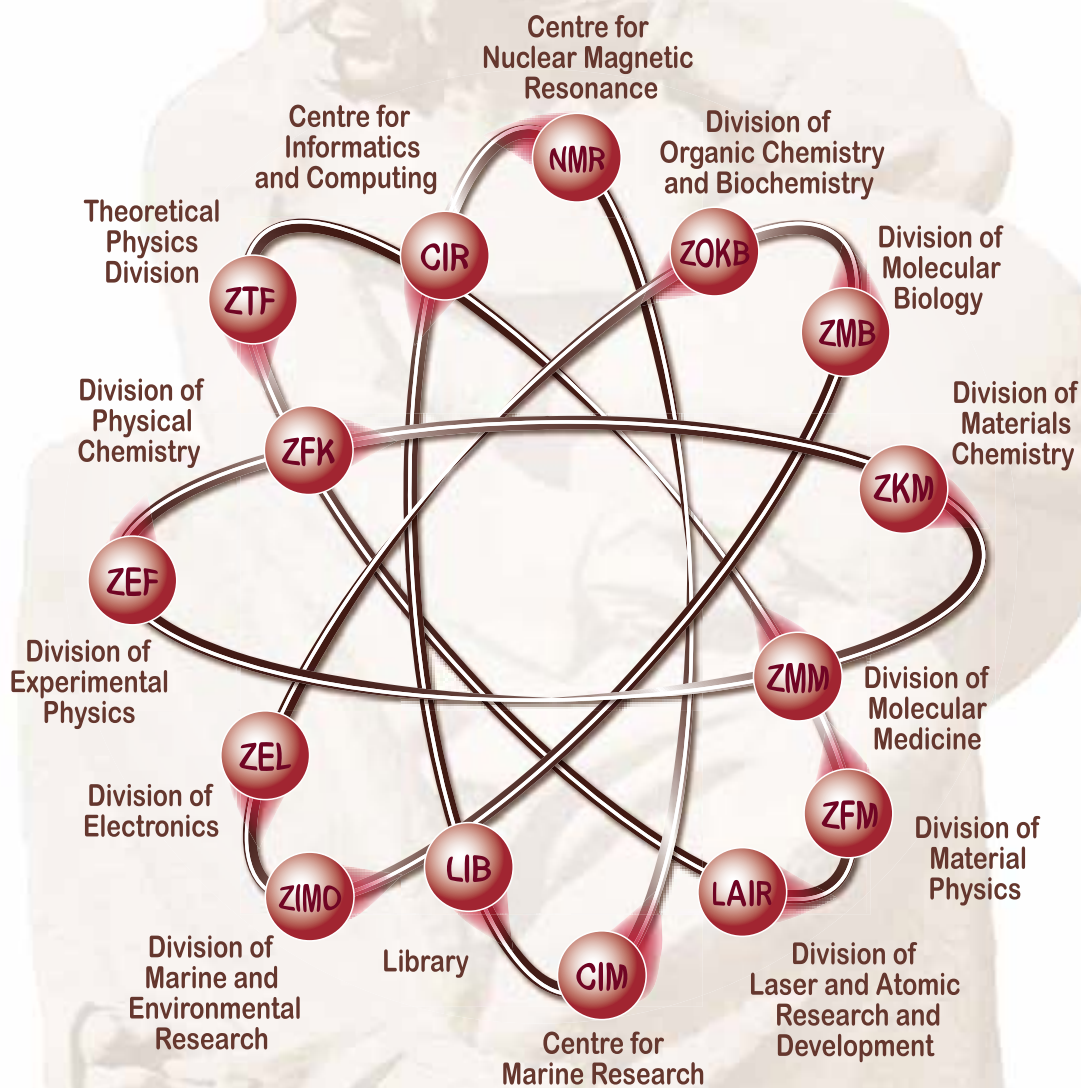
The portfolio of Rudjer Innovations contains more than 80 innovations and scientific projects in various fields with commercial potential but primarily in chemistry, medicine, biology, physics and informatics. Some have already been applied in industry and economy, and others have been prepared for various methods of commercialisation, depending on the interest and needs of buyers and partners. Besides its portfolio of innovations, Rudjer Innovations works on strengthening the cooperation between Ruđer Bošković Institute and companies from various business areas. RBI's know-how, professionalism and multidisciplinary approach in solving problems of all kinds represent a great potential for cooperation with companies.

The Rudjer Innovations database of innovations, projects and spin-off companies is available at a click of the mouse at web page www.r-i.hr.

Expansion

Rudjer Innovations began its existence in 2006 with a single employee, 1 project,

1 patent application, and 1 licence. By the end of 2008, it had expanded significantly to the point where now it has 7 employees, more than 80 projects (32 from outside RBI), 32 patent applications in different protection stages with 16 more to come, 7 licence agreements, 1 patent granted and 3 spin-off companies. The company employees made contacts with more than 100 companies from Croatia and abroad. It is planned to continue this expansion in 2009 through the establishment of additional spin-off companies, the addition of new innovations to the portfolio and the intensification of the connection between Croatian science and industry. By doing so, the principle aim is to establish RI as a regional leader in the area of commercialization of science and technology. Other key aims include: becoming the leading organisation for assessment, protection and commercialisation of intellectual property in Croatia; creating and becoming the central part of a network of researchers, entrepreneurs, business communities, banks and investors whose mutual goal is to ensure optimum commercialisation of intellectual property; and finally, increasing the number of activities and ensuring funding and support for future research and continuous innovations development as well as additional funds for rewarding inventors.





Ruđer Bošković Institute

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. World-wide, the RBI collaborates with many research institutions and universities upholding the same values and vision.