

Ruđer Bošković Institute

Annual Report 2011



The graphic features a dark blue background with a grid pattern. In the center, there is a circle of twelve yellow stars, similar to the European Union flag. To the right, there is a white silhouette of a person sitting and reading. In the bottom right corner, there is a logo for the Seventh Framework Programme, consisting of three blue horizontal bars of increasing length, with the text 'SEVENTH FRAMEWORK PROGRAMME' below it.

CLUNA - ZEF - Soić	NanoPV - ZFM - Pivac
UNCOSS - ZEF - Obhodaš	AIS-DC - CIR - Skala
HadronPhysics2 - ZEF - Supek	OpenAIREplus - KNJIŽ - Macan
SPIRIT - ZEF - Jakšić	STRAVAL - ZEF - Obelić
SOWAEUMED - ZEF - Obelić	EDA-EMERGE - ZIMO - Ahel
PARTICLE DETECTOR - ZEF - Antičić	Core Shell - CIM - Batel
e-LICO - ZEL - Šmuc	FoC II - ZTF - Zlatic
ENSAR - ZEF - Jakšić	BIOMINTEC - CIM - Batel
ECOFUN-MICROBIODIV - ZIMO - Petrić	

Zagreb, 2013.

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Dear reader,

Welcome to the 2011 Annual Report of the Ruđer Bošković Institute. The aim of this report is to provide a succinct overview of the most important activities and top achievements made at the Ruđer Bošković Institute during 2011. As such, the report covers exemplary performance in high-quality fundamental research, published in top journals or scientific books, and shows the strong involvement of scientists of the Ruđer Bošković Institute in higher education. The report also highlights selected awards, recognitions, patents, domestic and international projects and collaborations, important invited lectures, and international conferences organized by the Institute during the year.

On behalf of the Editorial Board, I would like to take this opportunity to sincerely thank the RBI staff for their cooperation during the preparation of this report. We would also like to thank you, the reader, for your interest and take pleasure in inviting you to share with us your comments and suggestions regarding future editions of this report.

Editor
Nela Pivac

Introduction

OVERVIEW

The year of 2011 saw the Republic of Croatia and Ruđer Bošković Institute (RBI) celebrate the 300th anniversary of the birth of the scientist visionary who is its namesake - Ruđer Josip Bošković, one of the greatest and most famous Croatian philosophers and scientists. The Croatian Parliament proclaimed the Year of 2011 as The Year of Ruđer Bošković in Croatia. One of the messages emerging from this important anniversary is that excellence and multidisciplinary in science and education must be constantly fostered, thereby creating value in all segments of society. In this sense, Ruđer Bošković is an excellent role model for today. Proudly bearing the name of this great scientific figure, the Ruđer Bošković Institute is regarded as Croatia's leading scientific institute in the natural and biomedical sciences as well as marine and environmental research, owing to its size, scientific productivity, international reputation in research, and the quality of its scientific personnel and research facilities. The Institute is the leading and most internationally competitive Croatian institute by virtue of its participation in international research projects, such as the IPA, IAEA and FP7 program funded by the European Commission, NATO, Cogito, COST, UNESCO and other international scientific foundations. While the RBI constitutes only about 6% of the total scientific community in Croatia, about 30% of the scientific papers and total scientific activities originate from its employees.

There are nearly 900 persons employed at the Institute today. Over 550 of them are scientists and researchers that pursuing research in more than 80 laboratories in theoretical and experimental physics, material

physics and chemistry, electronics, physical chemistry, organic chemistry and biochemistry, molecular biology and medicine, marine science and the environment, information and computer sciences, laser and nuclear research and development.

In addition to basic research, the RBI is strongly involved with the development of innovative research, participation in higher education and increasing public awareness of the importance of knowledge and science in modern society. These tasks are conducted in cooperation with universities, scientific institutes and other similar institutions in Croatia and all over the world. The Institute's experimental equipment, expertise in the fundamental sciences, and information and computer services maintain a high scientific standard and encourage the acquisition of new skills, which are important to the future of science and the transfer of technology in the economic sector.

Ruđer Josip Bošković, one of the greatest and most famous Croatian philosophers and scientists (1711-1787), was born in Dubrovnik, where he was educated at the Jesuit Collegium. He was a member of the Royal Society of London, the St. Petersburg Academy and Accademia dell'Arcadia, a corresponding member of the French Royal Academy of Sciences and a professor at many European universities. The highly delicate task of repairing cracks in the cupola of St. Peter's Basilica in the Vatican was entrusted to R. Bošković, confirmation that he was regarded as a leading European authority in static computations and civil engineering. At the request of Empress Maria Theresa of Austria, Bošković solved the problem of the stability of the Royal Library (now the National Library) in Vienna. He was also the founder of the Brera Astronomical Observatory near Milan. Bošković's

theory of forces anticipated modern physics by almost two centuries.

ORGANIZATION OF THE INSTITUTE

Organizationally, the RBI consists of twelve divisions, two centres, a library, the office of the Director General, as well as sections for maintenance and technical services and administration (Figure 1).

The administrative structure of the Institute sees central roles for the Board of Governors, the Director General and the Scientific Council. Important input is derived from the Heads of the Divisions and Centres (via their Divisional Councils), the Assistant Directors, as well as the Heads of the Administration, the Maintenance and Technical Services and the Library (Figure 2). The International advisory board provides vital external advice and guidance.

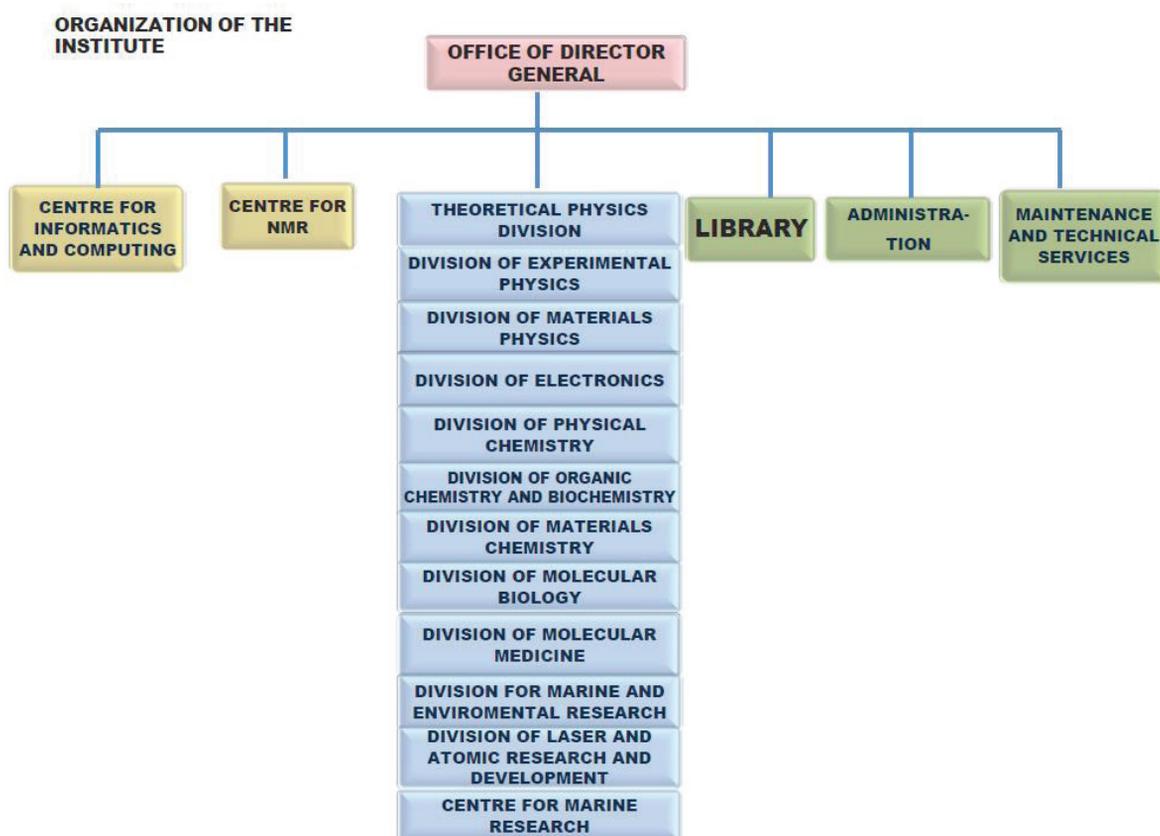


Figure 1. The organizational structure of the RBI

ORGANIZATIONAL SCHEME

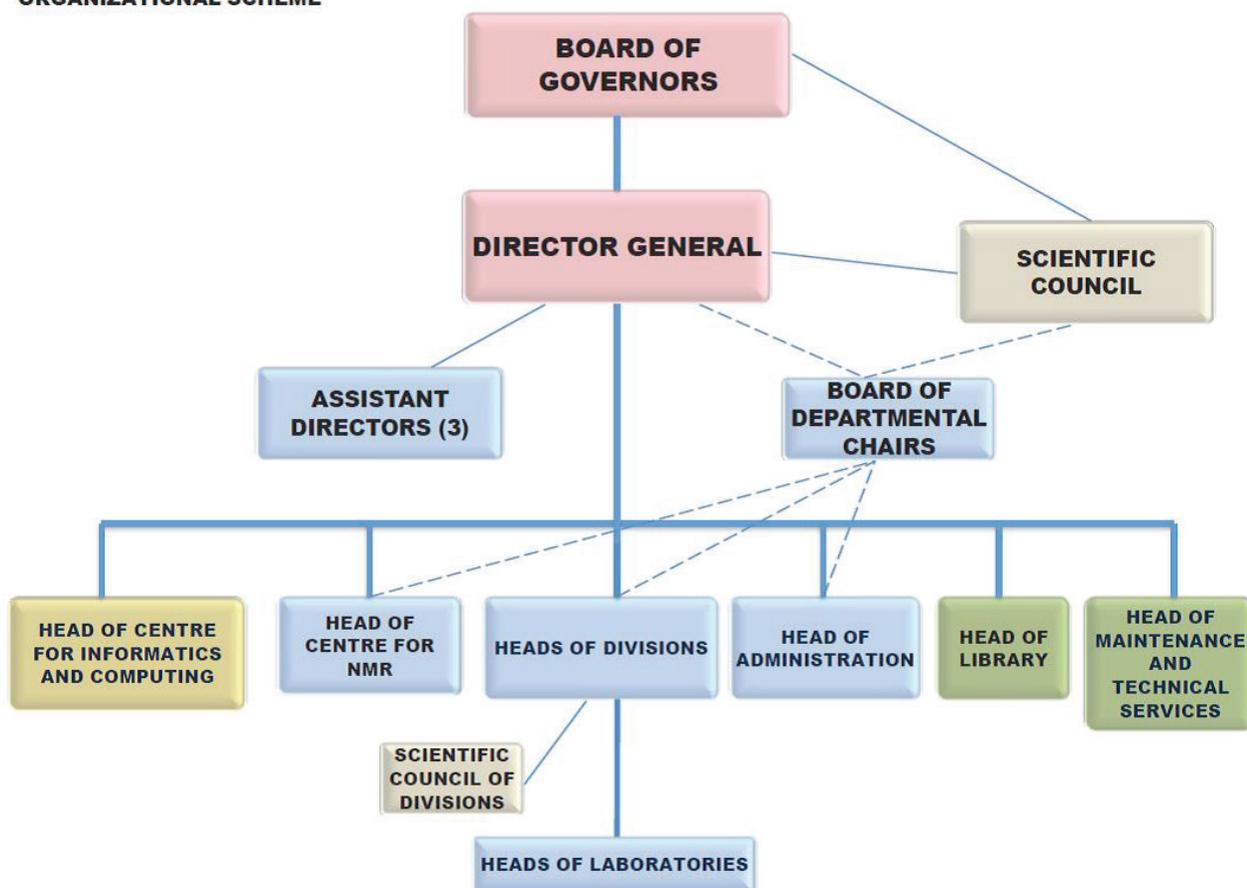


Figure 2. The administrative structure of the RBI

Director General: Danica Ramljak
 Head of the Scientific Council: Neven Bilić
 Chairman of the Board of Governors:
 Slavko Krajcar

International Scientific Board:

Jean-Marie Lehn, Laboratoire de Chimie
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 Fernando Azorin, Institute of Molecular Biol-
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 ence, USA
 Egon Matijević, Clarkson University,
 USA
 Jutta Ludwig Müller, Institute of Botany,

Technische Universität Dresden, Germany
 Werner E.G. Müller, Johannes Gutenberg Universität, Germany
 A.R. Peaker, University of Manchester, UK
 Roberto D. Peccei, University of California Los Angeles, USA
 Olivia Pereira-Smith, UT Health Science Center, USA
 Nadia Pinardi, University of Bologna, Italy
 Bogdan Povh, University of Heidelberg, Max-Planck-Institut für Kernphysik, Germany
 Miroslav Radman, Université René Descartes-Paris V, France
 Joseph Schlessinger, Yale University, USA
 Hans Joachim Seitz, Universität Hamburg, Germany
 Peter J. Stambrook, University of Cincinnati Medical Center, USA
 Rudolf Zechner, Institute for Molecular Biosciences, Austria
 Walter Giger, Swiss Federal Institute for Aquatic Sciences and Technology, Switzerland

ACTIVITIES

Fundamental research

The total number of research articles published by RBI scientists in 2011 was 679. Among these, 520 were published in journals cited by Current Contents, the majority of which were published in high ranking international Journals.

The details of the many important discoveries made by RBI scientists in 2011 are to be found in the subsequent sections of this report. Nevertheless, we present here a small section of highlights in order to convey a general impression of the kind research carried out at the Institute.

In a year of 2011, four RBI scientists had papers published within the highly prestigious Nature Publishing Group.

Marijan Ahel, from the Laboratory for Analytical Chemistry and Biogeochemistry of Organic Compounds in the Division for Marine and Environmental Research was a co-author of an article entitled: *The structure and catalytic mechanism of a poly(ADP-ribose) glycohydrolase*, which was published in the prestigious journal Nature. In the article, the crystal structure and mechanism of PARG are described for the first time. This discovery, in addition to its great fundamental significance, also provides a potential methodological advantage in finding a PARG inhibitor that could be used in the treatment of some diseases such as breast and ovarian cancers.

After appearing on the cover of Nature in 2010, this year Tomislav Domazet-Lošo, from the Laboratory of Evolutionary Genetics, Division of Molecular Biology, together with Diethard Tautz from the Max Planck Institute for Evolutionary Biology wrote an article entitled: *The evolutionary origin of orphan genes*, which was published in Nature Reviews Genetics. The authors demonstrate that the de Novo formation of genes from non-coding parts of a genome is an important evolutionary mechanism. According to the authors, the spontaneous generation of new genes, which have completely unique sequences, represents a mechanism that has functioned throughout all evolutionary epochs and is not peculiar only to the early emergence of life on earth 3.5 billion years ago.

Enis Afgan from the Optoelectronics and Visualisation Laboratory in the Centre for Informatics and Computing published an outstanding scientific article entitled *Harnessing cloud computing with Galaxy Cloud* in the journal Nature Biotechnology. The results facilitate simple access to an environment for performing bioinformatic analyses on a Cloud infrastructure using the Galaxy Web Application, which enables the creation and composition of analyses in the natural sciences and assures accessible, repeatable and transparent

computer searches. Galaxy Cloud, developed within the CloudMan project, allows individual researchers using a web browser, without any installations or configurations whatsoever, to access the complete infrastructure necessary for desired analyses, such as, for example, large BLAST searches or de novo genome sequencing.

Tin Klanjšček from the Laboratory for Informatics and Environmental Modelling in the Department for Marine and Environmental Research, together with colleagues from University of Alberta, Canada, published a paper entitled: Predicting climate change impacts on polar bear litter size, in Nature Communications, an online-only, multidisciplinary journal

DEPARTMENT	STAFF Research staff**	ARTICLES ^[1]				Books	Patents	THESES			
		Articles in CC journals	Articles in other journals and chapters in books	Articles in conference proceedings	Total articles			Ph. D. Theses (written by RBI staff)	Theses (mentored by RBI staff)		
									Ph.D.	M.Sc.	B.Sc.
Theoretical Physics Department	25	21	1	3	25				4		
Department of Experimental Physics	50	145	17	4	166			1	3	2	
Department of Materials Physics	27	39	3	9	51				2	3	
Department of Laser and Atomic Research and Development	7	16		4	20			1	2		
Department of Electronics	10	4	3	4	11						
Department of Physical Chemistry	40	54	8	3	65			1	1	2	
Department of Organic Chemistry and Biochemistry	60	61	6	2	69	1	1	4	7	10	
Department of Materials Chemistry	43	40	3	11	54			1	1		
Department of Molecular Biology	64	39	9	2	50	1		4	7	14	
Department of Molecular Medicine	67	65	14		79			5	11	13	
Department of Marine and Environmental Research	80	61	13	19	93		1	3	4	4	
Centre for Marine Research	39	26	2	1	29					1	
Centre for Informatics and Computing	6	1	1	14	16						
Centre for Nuclear Magnetic Resonance	10	17	12	2	31				4	1	
Library		1	1		2			1			
TOTAL RBI	528	520	89	70	679	2	2	21	42	53	1

[1] Original scientific papers and review papers in journals/conference proceedings and chapters in books.

** Scientists, post-doctoral fellows and graduate students

Table 1. Review of publications for the year 2011

dedicated to publishing high-quality research in all areas of the biological, physical and chemical sciences.

Darko Orešković from the Laboratory for Neurochemistry and Molecular Neurobiology in the Division of Molecular Biology, Ruđer Bošković Institute, together with Marijan Klarica of the School of Medicine at the University of Zagreb, published a review article entitled *Development of hydrocephalus and classical hypothesis of cerebro-spinal fluid hydrodynamics: facts and illusions* in the distinguished journal *Progress in Neurobiology* which is among the top 5% of journals in the field of neuroscience. In the paper, the classical hypothesis of the origin of hydrocephalus established a hundred years ago, which represents the textbook knowledge of medical students, neurologists, neurosurgeons and pathologists, is refuted by the authors, based upon their previously published research results. This paper by Drs. Orešković and Klarica proposes a new and different concept based upon experimental work, thereby opening new possibilities for discovering the cause of certain pathological conditions, primarily hydrocephalus, and potential new approaches to their treatment.

RBI scientists: Ivica Kopriva, from the Laboratory for optics and thin films in the Division of Laser and Atomic Research and Development, Mirko Hadžija, Marijana Popović-Hadžija and Marina Korolija from Laboratory for molecular endocrinology and transplantation in the Division of Molecular Medicine, together with Andrzej Cichocki, RIKEN, Japan, published a paper: *Rational Variety Mapping for Contrast-Enhanced Nonlinear Unsupervised Segmentation of Multispectral Images of Unstained Specimen* in the *American Journal of Pathology*, the leading journal in pathology research. The paper presents a method for enhancing the contrast of the multispectral images of a histopathological specimen of an algorithm of nonlinear segmentation. On two experimental unstained specimens, contrast was achieved comparable to that of a stained specimen. With further refinement, it should be possible to develop methods for the non-

linear segmentation of multispectral images, which would eliminate the need for staining in clinically important applications.

Dražen Vikić-Topić and Dejan Plavšić from the Laboratory for NMR Spectroscopy and Modelling in the NMR Centre, together with co-authors Milan Randić and Jure Župan, from the University of Ljubljana and Alexander T. Balaban from the Texas A&M University at Galveston, USA, published a paper entitled *Graphical Representation of Proteins* in the journal *Chemical Reviews*. *Chemical Reviews* is the most widely cited journal of the American Chemical Society, with an impact factor of 36 and also the first among the 140 journals in the category of Chemistry. The graphical representation of biosequences has been a subject of research in Bioinformatics for a quarter of a century, with particular momentum during the past ten years provided by our researchers.

Projects and other revenue

The RBI has 133 projects in basic research, which are funded by the Ministry of Science Education and Sport. Additional domestic competitive projects are provided by the Croatian Science Foundation and the Unity Through Knowledge Fund (UKF), from which RBI has 13 active projects, collectively. The Institute is involved with almost 100 international projects (including 15 FP7, 2 IPA, 8 IAEA, 2 NATO, 1 COST, 1 UNESCO, 1 SCOPES, and 59 bilateral projects), as well as around 50 applied and technological contracts (including 2 HRZZ, 1 HIT and 2 BICRO). The total financial value of these projects can be seen in Table 2, as well as the funding trends since 2007.

Table 2 also shows that the largest non-competitive source of revenue continues to be derived from the Ministry of Science, Education and Sports, which directly contributed almost € 22 M in 2011. A significant part of this revenue is dedicated to staff salaries (ca. 75%), while the remainder is related to various running costs. This so-called block grant

REVENUE	2007	%	2008	%	2009	%	2010	%	2011	%
Funding from the Ministry of Science, Education and Sports (MSES)	23.770,52	83,61%	25.755,01	86,37%	24.030,18	83,82%	23.372,73	81,61%	21.628,32	87,40%
National projects funding (Croatian Science Foundation, Croatian Institute of Technology, etc.)	1.017,19	3,58%	487,601	1,64%	345,916	1,21%	1.365,29	4,77%	941,694	3,81%
International projects funding (FP, NATO, IAEA, etc.)	1.377,93	4,85%	910,305	3,05%	1.575,53	5,50%	1.780,55	6,22%	1.042,51	4,21%
Commercial contracts	1.999,84	7,03%	2.449,66	8,22%	2.416,48	8,43%	1.873,09	6,54%	1.116,29	4,51%
Donations and other funding	264,046	0,93%	216,622	0,73%	300,392	1,05%	246,147	0,86%	16,619	0,07%
TOTAL	28.429,53	100%	29.819,20	100%	28.668,50	100%	28.637,81	100%	24.745,43	100%

Table 2. RBI Revenue from 2007-2011 (€)

was reduced in 2010. The total RBI revenue was reduced by almost € 3 M in comparison to 2010.

Organization of international **conferences and outreach activities**

As in previous years, the RBI continued to support the organization of numerous international and domestic conferences. Many of them were organized as a part of a series of events celebrating the 300th Anniversary of the birth of Ruđer Josip Bošković.

For example, two international symposiums were organized to celebrate this jubilee in May.

An international scientific symposium, *From Ruđer Bošković to Today: Contribution of Croatian Scientists to the World Scientific Heritage*, was jointly organized by the Ruđer Bošković Institute, City of Dubrovnik and Diocesan Secondary School Ruđer Bošković in Dubrovnik (formerly Jesuit Collegium Ragusinum attended by young Bošković). A symposium was held in Dubrovnik, under

the auspices of the President of the Republic of Croatia and the Prime Minister of the Republic of Croatia, and it featured lectures by renowned scientists: Ivo Šlaus, Rolf Heuer, Daniel Denegri, A. J. Stewart Smith, Goran Senjanović, Ivica Kostović, Paško Rakić, Boro Dropulić, Reshef Tenne, Vlasta Bonačić Koutecky, Tonica Valla, Davor Pavuna, Miroslav Radman, Brenda Andrews, Igor Štagljar, Davor Solter, Branimir Šikić, Hedvig Hricak, Siniša Volarević, Dmitrij Krainc, Slobodan Vukičević, Zlatko Bačić, Goran Ungar, Vladimir Hlady, Branko Ruščić, Werner E. G. Müller, Ivica Martinović and Nobel prize Laureate Carlo Rubbia.

The international symposium Ruđer Josip Bošković – Physicist and Astronomer was organized by the Ruđer Bošković Institute in a collaboration with the University of Zagreb, under the auspices of the Croatian Academy of Sciences and Arts and it was held at the Chemistry Department, Faculty of Science, University of Zagreb. It gathered renowned Croatian and international distinguished experts in the life and work of Ruđer Bošković: Mladen Martinis, Vincenzo Aq-

uilanti, Ksenofont Ilakovac, Luca Guzzardi, Ivica Martinović, Edoardo Proverbio and Ivo Šlaus who spoke about various aspects of his activities. On that occasion RBI initiated a new series of lectures dedicated to one of the greatest and most famous Croatian philosophers and scientists, entitled the Ruđer Bošković Lectures. A Nobel Laureate in Chemistry, Professor Jean-Marie Lehn, delivered the first lecture in the series: *Towards Complex Matter: Chemistry? Chemistry!*



Figure 3. Ruđer Josip Bošković Exhibition, Dubrovnik

In June, a group of researchers from the RBI's Laboratory for Radiation Chemistry and Dosimetry organized a workshop on *Free Radicals in Chemical Biology*. A workshop was held at the Ruđer Bošković Institute within the framework of the program of European Cooperation in Science and Technology – COST. The workshop gathered scientists from 47 research groups and 22 countries.

In July, the RBI organized an event for young researchers entitled *Scientific Encounters of the Third Kind*. During the two days of meeting, over 150 young researchers presented their research results in the fields of biology, molecular medicine, physics, chemistry, nanosciences, environment and oceanology through popular scientific lectures and poster presentations. The goal of this educational event was to encourage communication, competitiveness and scientific collaboration among young scientist in a various fields, as well as to stimulate the exchange of ideas and to promote multidisciplinary scientific research.

In September, RBI's Centre for Marine Research in Rovinj organized *46th European Marine Biology Symposium - EMBS*, the largest symposium of its kind in Europe. This is the second time that one of the most important symposia in the field of marine biology has been held in Rovinj, 40 years after the first. During the five days of the symposium, over 100 researchers worked actively on solutions that will contribute to the field of marine biology and raise awareness of the need for proper management of the seas and coasts. Both of these topics are very current in the politics of the European Union, which has issued a number of initiatives and directives on the conversation of the sea and marine diversity. Since Croatia is close to accession to the EU, its goal is to participate as much as possible in the implementation of these directives.

In October RBI organized two international events. A seminar entitled *Radiation Methods in the Protection of Cultural Heritage Artefacts*, was organized by the RBI's Radiation Chemistry and Dosimetry Laboratory and the Croatian Conservation Institute. The goal of the seminar was to familiarize conservators, conservator-restorers, curators and all professionals involved in the maintenance, preservation and presentation of cultural heritage artefacts, as well as owners and users, with methods that employ radiation. The Division of Experimental Physics of the Ruđer Bošković Institute hosted the NA61 collaboration meeting. NA61 is a large acceptance Hadron spectrometer with excellent capabilities for momentum, charge and mass measurements. The meeting hosted about 40 physicists from all over Europe that discussed about the latest NA61 results, future plans, NA61 silicon vertex and the role of the RBI experimentalists in its design, construction and implementation.

With the support of the Croatian Academy of Sciences and Arts, in September RBI have organized a symposium on the occasion of the 80th anniversary of the birth Nikola Cindro, founder of the RBI's Nuclear

Physics Laboratory. As a scientist, lecturer and an initiator of the internationally recognized Zagreb school of heavy-ion physics, Nikola Cindro contributed significantly to the recognition of the Ruđer Bošković Institute and Croatia in Europe and the world.

A DAQ/FPGA workshop was organized at the RBI in November as part of the Particle Detectors FP7 project. The purpose of this workshop was to present a practical introduction to modern DAQ systems and related hardware, with an overview. A number of foreign invited lecturers shared their specialized know-how. The focus was on, among other aspects, developments related to the future FAIR facility in Darmstadt, Germany, for which novel DAQ systems are being developed. The skills gained will be of use in all modern large nuclear, particle and astroparticle experiments.

In addition to the organization of various scientific events, during the 2011, RBI hosted numerous distinguished guests including the President of the Republic of Croatia Ivo Josipović. A Ceremonial Session of the Scientific Council of the RBI was held in President Josipović's honour. President Josipović described the RBI as the archetype of science for his generation and noted that science is the engine for the successful development of every country. "There is no progress without people of vision," he said, adding that responsible science must have general social and moral consequences. The President of the Republic also said that the Ruđer Bošković Institute can and should be the engine for the development of the Croatian society.



Figure 4. SCI-CSI Film Team

The year 2011 will be remembered by one truly a refreshing event in the Croatian scientific world. RBI's experimental physicists made a feature film - entitled SCI CSI. The plot turns around an investigation by an inspector and his associate of a murder that occurred at the RBI. After the experimental physicists offer their assistance and laboratories in the investigation, everything goes downhill. Approximately twenty RBI scientists have parts in the film, which was directed by research fellow Deša Jelavić Malenica, who also wrote the script.

Awards and Recognition

As in previous years, the achievements of RBI scientists were also recognized through numerous awards.

RBI scientists emeritus Biserka Kojić-Prodić and a senior research scientist from the Division of Theoretical Physics Nevenko Bilić received State Awards for Science. The Lifetime Achievement Award was presented to Biserka Kojić-Prodić, in recognition of her overall scientific research and exceptional contribution to the expansion of scientific knowledge and the application of results in the field of the natural sciences. Nevenko Bilić was presented the Annual State Science Award for scientific achievements in the area of the natural sciences and for his significant scientific contribution in the unification of dark matter and dark energy in quartessence models.

Young RBI scientists Irena Dokli, from Division of Organic Chemistry and Biochemistry, and Nives Ivić, from the Division of Physical Chemistry, received the Annual Award in the Field of Natural Sciences. Irena Dokli has published five scientific papers so far and competed with a study that describes the synthesis of N-protected azirdines with a detailed study of the mechanisms of the corresponding reactions, which was published in *Chemistry – A European Journal*. Nives Ivić has published three scientific papers to date and competed with a paper in which the biochemical mechanisms of aminoacyl-tRNA synthetase are in-

vestigated, particularly the truncated versions of the enzymes present in the genomes of various organisms. The paper was published in the prestigious journal PNAS.



Figure 4. Annual Award Laureates

Senior research scientist Saveta Miljanić, Division of Materials Chemistry was elected to the Council of the European Radiation Dosimetry Group - EURADOS. EURADOS is an association with the aim of advancing the scientific understanding and technical development of the dosimetry of ionizing radiation in the fields of radiation protection, radiology and medical diagnosis by stimulating collaboration among European laboratories. It was established in 1981 and today consists of 54 institutions from 24 countries as voting members and over 200 individuals as associate members.

Senior Scientist Maja Osmak, from the Division of Molecular Biology, received 100,000 HRK for Cancer Research in Croatia from Terry Fox Run Foundation. This donation is intended for studying cytostatic cancer therapies and especially for purchasing the necessary chemicals and equipment that are of great importance for the continuation of basic tumour research in the Laboratory for Genotoxic Agents.

Over thirty RBI scientists received RBI Annual Awards for the publication of one or more papers with a high impact factor, obtaining an international or domestic research grant of over 500,000 HRK or a project of exceptional importance to the RBI, an international patent or for scientific work included in the National Science Awards. Awarded scientists achieved important results in physics, chemistry, biomedicine and molecular biology. They pub-

lished papers in the leading journals in these fields and received significant funding within the FP7 and other international and domestic competitive projects.

Education

Although the RBI is currently not able to conduct its own, independent postgraduate study program, it has developed collaborations with several universities in Croatia through a number of doctoral and specialist study programs. In addition, through basic agreements with various universities in Croatia, RBI scientists actively participate in programs of higher education in Croatia. Owing to the large number of potential mentors and qualified researchers, as well as the relatively modern research equipment, the RBI remains an attractive place for the best students from Croatian universities to pursue doctorates, which continue to provide an influx of qualified doctoral candidates. Table 3 and Figures 6 and 7 provide an overview of the level of courses and their distribution across different locations and Divisions, respectively.

Type of course	Number of courses
Undergraduate courses	86
Graduate courses	33
Ph.D. courses	187
Additional specialist courses	9
Total	315

Table 3. Number of the courses held by RBI staff in 2011.

In the year 2011 Ruđer Bošković Institute and the Faculty of Chemistry and Technology, University of Split, initiated a joint doctoral program in Chemistry of the Mediterranean Environment, which will meet the need for doctoral studies in the natural sciences in the field of chemistry at the University of Split. The proposed doctoral program is comparable to the programs of the University of Zagreb, in particular the Faculty of Chemical Engineering and Technology and the Faculty of Science, as well as distinguished European

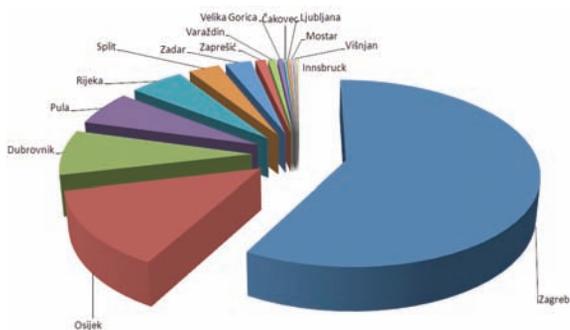


Figure 6. The distribution of the RBI courses by the location of the relevant hosting institution

universities in neighbouring countries such as the University of Geneva, Switzerland; the University of Vienna, Austria; the University of Ljubljana, Slovenia, and the University of Belgrade, Serbia.

Intellectual Property

Apart from fundamental research and education, the activities of the RBI also result in various forms of intellectual creations. One important aspect of the RBI's mission is the protection of intellectual property and its commercialization. In this context, various specific activities have been initiated and realized over the last few years. As a subsidiary, the Ruđer Bošković Institute established Ruđer Innovations Ltd., a company specializing in the commercialization of innovations and technology transfer. The intellectual property portfolio of Ruđer Innovations includes innovations protected by patents or patent applications in various fields of science that have commercial potential. In 2011 RBI was granted three patents.

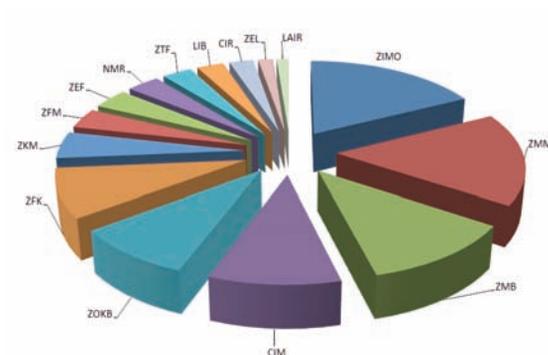


Figure 7. The distribution of the RBI courses by RBI Division

The State Intellectual Property Office of the Republic of Croatia granted a patent for the innovation "N,N',N" -Tris-(3-dimethylaminopropyl)-guanidine: the procedure of preparation from carbodiimide and application in reactions of the transesterification of oil" to the inventors Mirjana Eckert-Maksić and Zoran Glasovac. The patent was published in The Croatian Intellectual Property Gazette no. 1/2011.

Following recognition by the United States Patent and Trademark Office, the European Patent Office (EPO) granted Patent No. 077000434.9 for a Mixed Bacterial Culture for Atrazine Degradation to Dubravka Hršak.

A group of researchers in the Department of Organic Chemistry and Biochemistry Nikola Basarić, Marija Alešković and Kata Majerski have been awarded a US patent. Patent number US 8,022.097 is entitled "Adamantane-dipyrrromethane Derivatives, Method of Preparation and Applications in Anion Sensing".

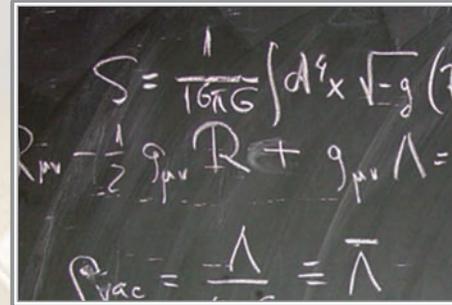


DIVISIONAL ORGANIZATION

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



nology and nanoscience. The members of the Division continued to be involved in lecturing at the University of Zagreb and the University of Split and a number of students completed their B. Sc., M. Sc. and Ph. D. theses.

OVERVIEW OF THE DIVISION

The research performed in the Theoretical Physics Division covers the theoretical investigation of high-energy physics, including heavy-quark physics, perturbative quantum chromodynamics, gravity, cosmology, and general and mathematical physics. There is substantial research activity in condensed matter physics, nanophysics and complex systems. Our strategic directions include research focussed on CERN related phenome-

TOP ACHIEVEMENTS

Graphene on Ir(111): Physisorption with Chemical Modulation

The large supercell of graphene adsorbed on an Ir(111) surface is clearly visible as a moiré pattern in STM experiments due to the small mismatch of the two periodicities,. An accurate theoretical modeling of the system requires DFT calculations with nonlocal van

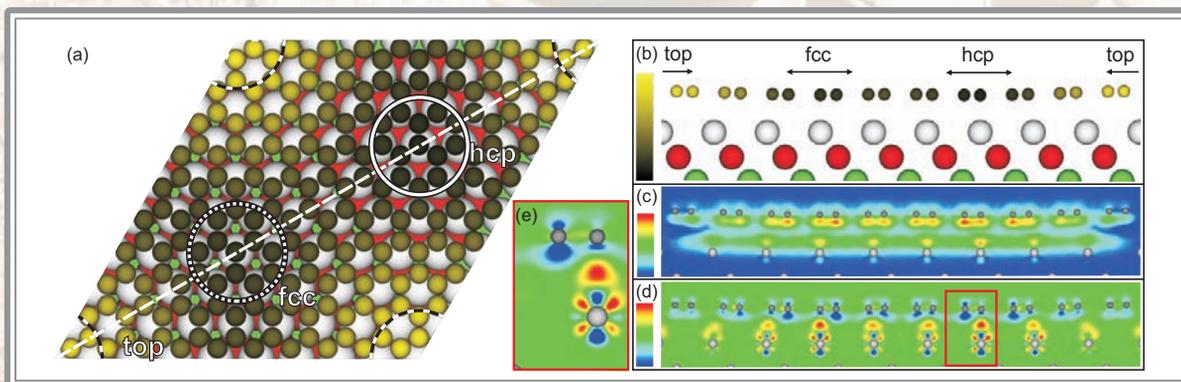


Fig. 1. Top and side view of the relaxed structure of graphene adsorbed on Ir(111) surface obtained by DFT calculations including vdW interactions. Also shown are the nonlocal correlation binding energy density caused by adsorption and the charge transfer upon adsorption.

der Waals correlation functional. We find bonding of graphene to Ir(111) to be due to the van der Waals interaction with an antibonding average contribution from chemical interaction (Busse et al., 2011).

On ultraviolet/infrared mixing in noncommutative gauge field theories

We studied the self-energy contribution for neutral massless fermions in the q-exact approach of NC QED. We show for the first time, by explicit calculation the equal-footing presence of ultraviolet divergence, softened ultraviolet/infrared mixing effects and finite terms in the NC neutrino propagator in closed form. All divergences can be eliminated for a unitary choice of the non-commutative parameter θ , however finite terms become responsible for extra modification of neutrino dispersion relation (Horvat et al., 2011).

Kappa-deformed Snyder space and Hopf algebra

Lie-algebraic deformations of Minkowski space with undeformed Poincare algebra, which interpolate between Snyder and kappa-Minkowski space are investigated. Realizations of non-commutative coordinates in terms of commutative coordinates and derivatives are found as well as the corresponding deformed Leibniz rule, the coproduct structure and star product. Particular cases, such as Snyder and kappa-Minkowski in Maggiore-type realizations are examined in detail (Meljanac et al., 2011).

Scalar field propagation in the ϕ^4 kappa-Minkowski model

A hybrid approach between standard quantum field theory and NCQFT on the κ -Minkowski spacetime, due to the anticipation of specifically κ -deformed statistics on the κ -Minkowski spacetime was developed.

Computed one loop quantum corrections, i.e. connected two-point Green's functions, show for the first time that the NC scalar field propagation is very different at different propagation energies. At the Planckian energies we obtain the direction dependent κ -modified dispersion, thus the massive scalar field shows a birefringence effect (Meljanac et al., 2011).

A Twisted look on kappa-Minkowski

Kappa-Minkowski space-time is an example of noncommutative space-time with potentially interesting phenomenological consequences. We constructed an action for the gauge and matter fields in a geometric way, and using the Seiberg-Witten map to relate non-commutative and commutative degrees of freedom we obtained first order corrections in the deformation parameter (Dimitrijević and Jonke, 2011).

Constraining non-commutative field theories with holography

Two theoretically important windows to quantum gravity phenomena at low energies: the non-commutative quantum field theories (NCGFT) and holography are connected for the first time via a specific form of ultraviolet/infrared mixing (NC scale) in NCGFT and via ultraviolet and infrared cut-offs in holography (Horvat and Trampetić, 2011).

Galaxy rotation curves without dark matter

For Renormalization Group corrected General Relativity theory the scale-setting procedure is applied to astrophysical systems. The choice of scale that reproduces the galaxy rotation curves without dark matter is derived for spherically symmetric systems with fluid with polytropic equation of state (Domazet and Štefančić, 2011).

Electrodynamics on kappa-Minkowski space-time

We derive Lorentz force and Maxwell's equations on kappa-Minkowski space-time up to the first order in the deformation parameter. It is shown that the motion in kappa space-time can be interpreted as motion in a background gravitational field, which is induced by this non-commutativity (Harikumar et al., 2011).

EDUCATION

In 2011, the members of the Division continued to be involved in lecturing at undergraduate and graduate courses mostly at the University of Zagreb (Faculty of Science, School of Economics and Management) and the University of Split (Faculty of Science, Faculty of Civil Engineering and Architecture). A number of students completed their B. Sc. and M. Sc. theses.

AWARDS

Nevenko Bilić received the Annual State Award of Croatia for achievements in science in 2010. Nevenko Bilić, Radovan Brako, Silvi-je Domazet, Branko Guberina, Larisa Jonke, Hrvoje Štefančić, Josip Trampetić and Vinko Zlatić received the RBI Director's Award for Scientific Excellence in 2011 and Larisa Jonke served as a member of the Steering Committee for the ESF research network Quantum Geometry and Quantum Gravity (July 2007 – December 2011).

PROJECTS

Programs supported by the Ministry of Science, Education and Sport

1. High energy physics, gravity and cosmology. Program leader: Branko Guberina

Projects supported by the Ministry of Science, Education and Sports

1. Surfaces and nanostructures: Theoretical approaches and numerical calculations, Radovan Brako
2. Electronic properties of hybrid nanostructures, Željko Crljen
3. Fundamental interactions in elementary particle physics and cosmology, Branko Guberina
4. Noncommutative spaces in high energy physics, Josip Trampetić
5. Matrix models, duality and field theory, Larisa Jonke
6. Quantum field theory, noncommutative spaces and symmetries, Stjepan Meljanac

Research, developmental and international project

1. The structures of higher order in the non-commutative standard model based on the Seiberg-Witten mapping and applications of the same particle physics at extreme energies, Josip Trampetić (National Science Foundation of Croatia)
2. Integrable systems and noncommutative structures, Zoran Škoda (Croatian-French Project in the program "COGITO" - partnership Hubert Curien)
3. Modified gravity theories and the accelerated expansion of the universe, Hrvoje Štefančić (Croatian-Serbian Bilateral Project)
4. Forecasting Financial Crises, Vinko Zlatić (EU FP7-ICT-255987 – FOC-II Project)

SELECTED INVITED LECTURES

1. Melić B, CP violation with the fourth generation quarks, Workshop „The Role of Heavy Fermions in Fundamental Physics“, Portorož, Slovenia, April 11-13, 2011
2. Andrašić A, QCD in the Coulomb Gauge, Austria-Croatia-Hungary-Triangle Workshop

- „Strong Interactions in Quantum Field Theory“, Furstenfeld, Austria, May 4-6, 2011
3. Škoda Z, Morphisms of noncommutative spaces, Workshop “Algebraic structures in mathematical physics”, Zagreb, Croatia, May 20-21, 2011
 4. Trampetić J, Photon-neutrino interaction in q-exact covariant NC field theory, Bayrischzell Workshop 2011: Noncommutativity and Physics: Spacetime Quantum Geometry, Bayrischzell, Germany, May 20-23, 2011
 5. Trampetić J, Photon-neutrino interaction in theta-exact covariant NCGFT: Phenomenology and quantum properties, XXIX Max Born Symposium: „Super, Quantum & Twistors II“, Wroclaw, Poland, June 28-30, 2011
 6. Škoda Z, Globalizing Hopf-Galois extensions, Workshop “Homological mirror symmetry and category theory”, Split, Croatia, July 11-15, 2011
 7. Bilić N, Supersymmetric dark energy, The SEENET-MTP Workshop BW2011 “Particle Physics from TeV to Plank Scale”, Donji Milanovac, Serbia, August 28 -September 1, 2011
 8. Jonke L, A Twisted Look on Kappa-Minkowski: U(1) Gauge Theory, The SEENET-MTP Workshop BW2011 “Particle Physics from TeV to Plank Scale”, Donji Milanovac, Serbia, August 28 - September 1, 2011
 9. Melić B, The puzzling $B \rightarrow PP$ decays, Workshop „Colour meets Flavor: Quantum Chromodynamics and Quark Flavour Physics“, University of Siegen, Siegen, Germany, October 13-14, 2011
 - Gerber T, Atodiresei N, Caciuc V, Brako R, N’Diaye A T, Blügel S, Zegenhagen J, Michely T. Graphene on Ir(111): Physisorption with chemical modulation. *Phys Rev Lett* **107** (2011) 036101.
 2. Meljanac S, Samsarov A, Trampetić J, Wohlgenannt M. Scalar field propagation in the ϕ^4 kappa-Minkowski model. *J High Energy Phys* **12** (2011) 010.
 3. Dimitrijević M, Jonke L. A twisted look on kappa-Minkowski: U(1) gauge theory. *J High Energy Phys* **12** (2011) 80.
 4. Horvat R, Ilakovac A, Trampetić J, You J. On UV/IR mixing in noncommutative gauge field theories. *J High Energy Phys* **1112** (2011) 081.
 5. Bilić N. Vacuum fluctuations in a supersymmetric model in FRW spacetime. *Phys Rev D* **83** (2011) 105003.
 6. Domazet S, Štefančić H. Renormalization Group scale-setting in astrophysical systems. *Phys Lett B* **703** (2011) 1.
 7. Horvat R, Trampetić J. Constraining noncommutative field theories with holography. *J High Energy Phys* **2011** (2011) 112.
 8. Harikumar E, Jurić T, Meljanac S. Electrodynamics on κ -Minkowski space-time. *Phys Rev D* **84** (2011) 085020.
 9. Groote S, Körner J G, Melić B, Prelovšek S. Survey of top quark polarization at a polarized linear $e^+ e^-$ collider. *Phys Rev D* **83** (2011) 054018.
 10. Meljanac S, Meljanac D, Samsarov A, Stojić M. Kappa Snyder deformations of Minkowski spacetime, realizations, and Hopf algebra. *Phys Rev D* **83** (2011) 065009.
 11. Zlatić V, Štefančić H. Model of Wikipedia growth based on information exchange via reciprocal arcs. *Europhys Lett* **93** (2011) 58005.
 12. Horvat R, Kekez D, Schupp P, Trampetić J, You J. Photon-neutrino interaction in theta-exact covariant noncommutative field theory. *Phys Rev D* **84** (2011) 045004.
 13. Andraši A, Taylor J C. Renormalization in Coulomb gauge QCD. *Ann Phys* **326** (2011) 1053.
 14. Meljanac S, Samsarov A. Scalar field theory on kappa-Minkowski spacetime and translation and Lorentz invariance. *Int J Mod Phys A* **26** (2011) 1439.

SELECTED ORGANIZED CONFERENCES

1. The Third Quantum Gravity & Quantum Geometry School, Zakopane, Poland, February 28 – March 13, 2011 (Larisa Jonke, member of the Scientific Organizing Committee)

SELECTED PUBLICATIONS

1. Busse C, Lazić P, Djemour R, Coraux J,



Chapters in books

1. Zlatić V. Knowledge Networks: The Case Of Wikipedia. Complex Networks, in Ency-

clopedia of Life Support Systems (EOLSS). Caldarelli, Guido (ed.). Oxford, UK, Eolss Publishers, 2011, pp 79-106.

FTZ

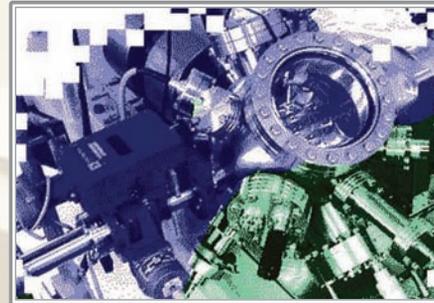


DIVISIONAL ORGANIZATION

Head: Tome Antičić

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

- ⇒ Laboratory for hadron physics, Ivan Supek
- ⇒ Laboratory for nuclear physics, Zoran Basrak
- ⇒ Laboratory for astroparticle physics, Raul Horvat
- ⇒ Laboratory for electromagnetic and weak interactions, Milica Krčmar
- ⇒ Laboratory for ion beam interactions, Milko Jakšić
- ⇒ Laboratory for measurement of low-level activities, Bogomil Obelić
- ⇒ Laboratory for high energy physics, Krešo Kadija
- ⇒ Laboratory for nuclear analytical methods (LNAM), Jasmina Obhodaš
- ⇒ Group for hadronic spectroscopy, Alfred Švarc



tion applications. The division has about 65 staff, including more than 30 PhDs. 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 non-MZOS sources, which was used, among others, to significantly enhance its experimental capabilities.

The main strategic objectives of the DEP for the next five years are briefly:

- A significantly enlarged experimental contribution in top large international physics collaborations, in particularly involving experimental work at the DEP site, leading to a much more prominent role in these experiments.
- Strengthened partnerships at numerous levels with prominent European institutions.
- Increased experimental capabilities and capacities for experiments at the local RBI Tandem accelerator facility.
- Additional focus on local experimental capabilities, such as the Cockcroft Walton accelerator (neutron generator), or the anticoincidence germanium system experiments.

OVERVIEW OF THE DIVISION

The core activities of the Division of Experimental Physics involve experimental ion beam, nuclear, particle and astroparticle physics, interdisciplinary research including nanotechnology, detector and sensor testing and development, as well as related radia-

- Development of an automated underwater vehicle, which integrates several sensors for detection and identification of objects lying on the sea floor.
- Improved characterization of advanced materials and their modification.
- Improved cooperation with partners, such as University of Zagreb, Split and Rijeka, Croatian industry, as well as local cultural institutions and authorities.
- Traditionally strong activities regarding development and applications of radiation based techniques in interdisciplinary research areas.
- Increased attraction for top Croatian students, as well as for current top staff.
- Increasing success rates in obtaining external funding.

TOP ACHIEVEMENTS

The Crystal Ball Spectrometer and Frozen Spin Polarized Target

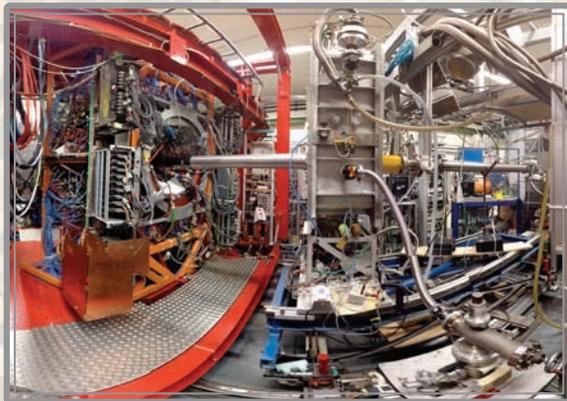


Fig. 1. Frozen Spin Target at MAMI.

During this year for the first time our Crystal Ball Collaboration at the Mainz Microtron (MAMI) successfully used both a transversely and longitudinally polarized target. RBI scientists have significantly contributed to the assembly and running of this new state-of-the-art Frozen Spin Polarized Target. This new target/detector setup enables investigation of many double polarization measurements for

the first time. So far the CB Collaboration has already published more than a dozen publications in high impact journals such as Phys. Rev. Letters, Phys. Lett. B, Phys. Rev. C and European Physical Journal.

Radiation hardness tests of semiconductor detectors

A novel experimental methodology of ion microbeam irradiation supported by a strong theoretical framework has been developed to study the effects of radiation damage in silicon (Pastuović et al., 2011). Since short irradiation time is needed to produce a high defect concentration in semiconductor detectors, a low cost IBIC (ion beam induced charge) methodology is very suitable for testing of radiation hard materials and particle detectors which are under development for high energy physics experiments in CERN and elsewhere.

Chemical speciation by $K\beta$ X-Ray Emission Spectroscopy

Crossover and valence band $K\beta$ x-rays of chromium oxides were measured by high resolution PIXE setup (Fazinić et al., 2011a). Measured results were used together with other available experimental data to perform parametrization of secondary contributions in $K\beta$ spectra of 3d transition metal oxides for chemical speciation and structural analysis of materials (Fazinić et al., 2011b).

Pionic fusion in light-ion systems

Pionic fusion is a highly coherent process in which two nuclei fuse to a united nucleus and the available centre-of-mass (C.M.) energy is emitted through the pion channel. The examined reactions ${}^4\text{He}({}^3\text{He},\pi^0){}^7\text{Be}$ and ${}^6\text{Li}({}^4\text{He},\pi^0){}^{10}\text{B}^*$ were performed at about 10 MeV above the coherent pion production threshold. Such reactions give specific insight into the role of pions in the nu-

clear interaction. A phenomenological study of the pion angular distributions has been performed and the results of this analysis confirm the importance of the clustering correlations for pionic fusion (see in Fig. 2). The mass dependence of the pionic fusion reaction is in agreement with the results of the existing models extrapolated to this reaction (Joulaeizadeh et al., 2011).

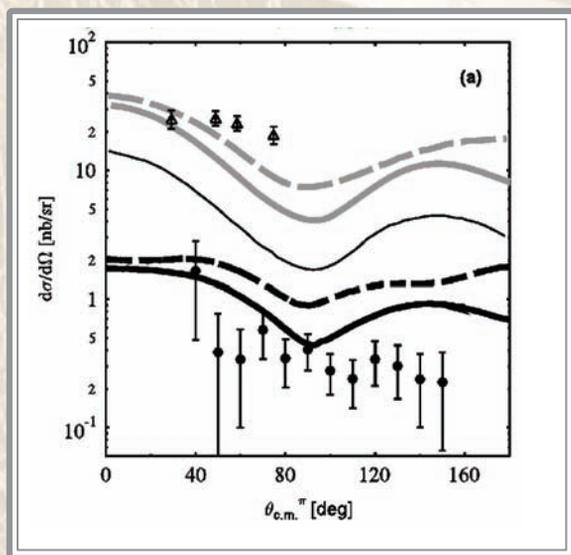


Fig. 2. Angular distribution of pionic fusion reaction cross section at subthreshold energies. Full circles are the results of this experiment for the ${}^6\text{Li}({}^4\text{He}, \pi^0){}^{10}\text{B}^*$ reaction, whereas triangles are for the ${}^4\text{He}({}^3\text{He}, \pi^+){}^7\text{Li}$ reaction. The thin black curve is the result of the cluster model for the ${}^4\text{He}({}^3\text{He}, \pi^0){}^7\text{Be}$ reaction. The thick grey and black curves are the results based on, respectively, the cluster and shell model for the ${}^4\text{He}({}^3\text{He}, \pi^+){}^7\text{Li}$ reaction.

Single and pair neutron transfers at sub-barrier energies

Multinucleon transfer excitation function in the ${}^{96}\text{Zr}+{}^{40}\text{Ca}$ system has been measured with unprecedented efficiency and resolution at and below the Coulomb barrier. The experimental data for one and two-neutron transfer channels have been compared with state of the art microscopic calculations. Experimental +2n transfer cross sections have been found to be enhanced by two orders of magnitude with respect to theoretical calculations when including the ground-to-ground state transitions. Part of this enhancement

has been explained by the excitation of the 0^+ state of ${}^{42}\text{Ca}$, whose wave function is dominated by the two neutrons in the $2p_{3/2}$ shell (see in Fig. 3). These features point to the presence of strong neutron-neutron correlations in heavy-ion-transfer reactions which may shed light on the presence of a nuclear Josephson effect (Corradi et al., 2011).

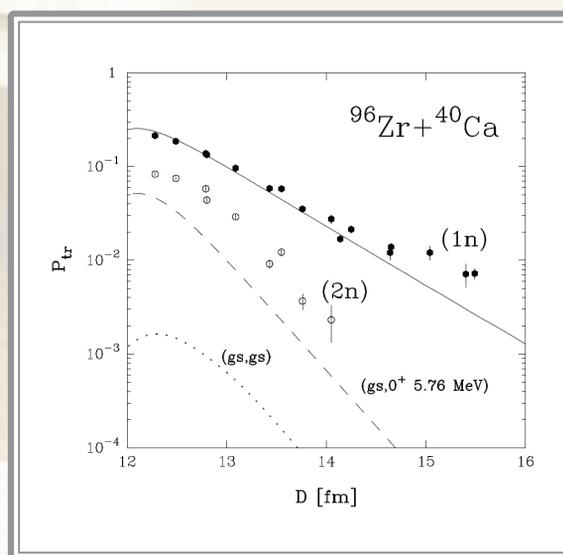


Fig. 3. Theoretical transfer probabilities for one- and two particle transfer (lines) in comparison with the experimental data (points). The full line represents the inclusive transfer probability for one-neutron transfer, the dotted line the ground-ground state transition for the two-neutron transfer, and the dashed line is due to the transition to the first 0^+ excited state at 5.76 MeV in ${}^{42}\text{Ca}$ and which strongly dominates the two-neutron transfer probability.

Search for solar axions

At CERN, a group of our scientists supervised the preparation and publication of a Physical Review Letters paper presenting the results of the search for sub-eV mass solar axions by the CAST experiment with ${}^3\text{He}$ buffer gas. The obtained limit on the axion-photon coupling constant excludes an important part of the theoretically favoured region (Arik et al., 2011).

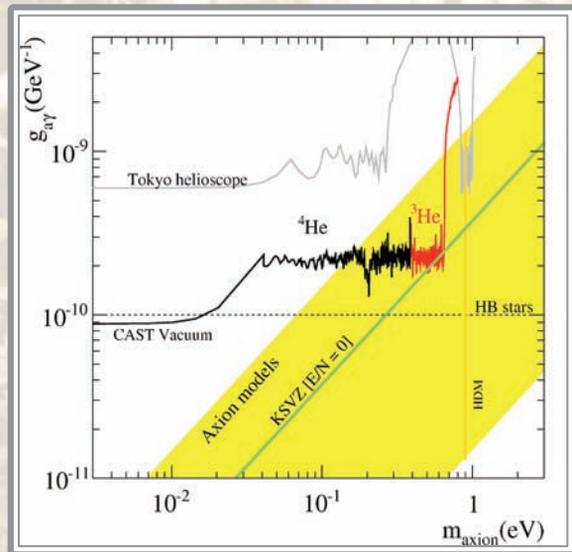


Fig. 4. Exclusion plot in the axion-photon coupling versus the axion mass plane achieved by CAST in the vacuum, ^4He , and ^3He phase. The yellow band represents typical theoretical models.

Full production mode for the Crystal Ball Collaboration with Hunting low-mass bosons from the Sun

In an experiment performed at RBI we searched for keV-mass bosons emitted from the Sun, by looking at a process analogous to the photoelectric/Compton effect inside the HPGe detector. The obtained limits tighten up constraints on non-Newtonian gravity much more efficiently than those obtained from the Casimir force measurements (Horvat et al., 2011a).

Within an approach in which noncommutative gauge theory can be realized as an effective quantum field theory, we require additional compliance with the holographic bounds. It was shown that such a “beefed up” theory is at odds with some experimental bounds (Horvat and Trampetić, 2011).

In the effective field theory approach to the Higgs inflation, it was shown the restriction to the UV cutoff coming from the scale of violation of the tree-level unitarity and that coming from the holographic bound are, in general, very hard to reconcile, especially for higher-dimensional operators (Horvat, 2011b).

First multiboson measurements at the Large Hadron Collider

The Large Hadron Collider (LHC) at CERN has started measuring proton proton collisions in 2010 at a center of mass energy of 7 TeV. After the first successful year of operation, LHC performance in 2011 surpassed all expectations and the LHC experiments have accumulated a large amount of data which allowed for a very good start on the exploration of the TeV energy range. The RBI group on the Compact Muon Solenoid experiment has played a leading role in some of the first electroweak measurements, involving heavy W and Z bosons. The focus of the group was on the physics of multibosons final states involving two or more electroweak gauge bosons in the final state. A member of the group was named editor and was leading the effort towards the first measurement of the Wg and Zg processes based on 36 inverse picobarns of data accumulated in 2010 and he was put in charge by the CMS Collaboration of all diboson processes measurements on 2011 data, while the graduate students of the group played a leading role in these analyses. The group produced the first measurement of the WZ final state at the LHC with CMS, and has contributed to the first search for anomalous triple gauge couplings in the WW and Wg processes. The group also started the direct exploration of new physics at the LHC and searched for new particles decaying into the WZ final state, as predicted in the context of new physics scenarios such as Technicolor or the Sequential Standard Model.

Plitvice Lakes investigation - environment and climate change

Influence of environment and climate change on the biologically induced calcite precipitation using isotopic, geochemical, SEM and TEM microscopy (Barešić et al., 2011).

Relevance of complex branch points for partial wave analysis

In collaboration with the KFK Juelich group we have investigated the existence and importance of complex branch points which naturally appear when a resonant state is formed in a three body final state. We were the first to demonstrate the existence of such branch points in the complex energy plane and then showed in the example of the $\pi N P_{11}$ partial wave that it is not possible to distinguish the structures induced by the latter from a true pole signal based on elastic data alone (Ceci et al., 2011).

Extraction of poles from a worldwide collection of partial wave amplitudes

Each and every energy-dependent partial-wave analysis parameterizes pole positions in a procedure defined by the way in which the continuous energy dependence is implemented, so they are inherently model-dependent. To reduce this model dependence, we use only one, coupled-channel, unitary, fully analytic method based on the isobar approximation to extract the pole positions from each available member of the worldwide collection of partial-wave amplitudes, which are understood as nothing more but a good energy-dependent representation of genuine experimental numbers assembled in the form of partial-wave data (Hadžimehmedović et al., 2011).

Stability of the Zagreb realization of the Carnegie-Mellon-Berkeley coupled-channels unitary model

We have used the Zagreb realization of the Carnegie-Mellon-Berkeley coupled-channel, unitary model as a tool for extracting pole positions from the world collection of partial-wave data, with the aim of eliminating model dependence in pole-search procedures. In order that the method makes sense, we dis-

cuss the stability of the method with respect to the strong variation of different model parameters. We show that the Zagreb CMB procedure is very stable with strong variation of the model assumptions and that it can reliably predict the pole positions of the fitted partial-wave amplitudes (Osmanović et al., 2011).

Accelerator provides Trans National Access (TNA) for european scientists

On the basis of availability of several unique beam lines for materials analysis and modification, the Management Board of the FP7 Project SPIRIT elected our Institute as a provider for Trans National Access (TNA) at its meeting in March 2011 at Farnham, UK. Within the TNA scheme, scientists from EU and associated states can apply for beam time at the RBI Tandem Accelerator Center. For successfully evaluated proposals, funding is secured through the SPIRIT project. During November the first three TNA experiments were completed. Experiments involved two groups from Italy (INFN Catania and Torino) and one from France (CEA Saclay).

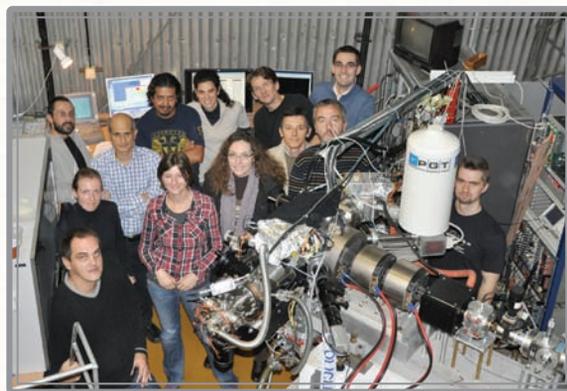


Fig. 5. The first TNA experiment proposed by Domenico Torressi (up left) concerned investigation of Si strip detector response using IBIC technique at the RBI microbeam facility.

NEW EQUIPMENT

New PIXE/RBS chamber for air pollution monitoring

Through the IAEA Project CRO8008: *Upgrades of nuclear analysis techniques for air pollution monitoring*, a new PIXE chamber has been installed at one of the beam lines of the 1.0 MV Tandatron accelerator (Figure 6).



Fig. 6. In addition to RBS (Rutherford Backscattering Spectrometry), the new chamber is equipped with two x-ray detectors optimized for analysis of light and heavy elements in air particulate samples using PIXE spectroscopy.

Upgraded dual irradiation beam MMRPC Barrel for ToF measurements of FOPI

For the FOPI-Collaboration detector at GSI, Darmstadt the new time-of-flight (ToF) barrel made of Multi-strip Multi-gap Resistive-Plate-Counters (MMRPC) was developed, tested and applied. The Barrel has an active area of 5m² and consists of 30 so-called super-modules (SM) made of 5 MMRPCs each (see Fig. 8) giving in total 2400 strips which are read out at both ends by custom-designed electronics. The obtained overall time resolution of the FOPI ToF system is better than 90 ps allowing increasing the Identification limit for charged kaons up to laboratory momenta of at least 1GeV/c (Kiš et al., 2011).

Since our collaboration also uses targets which do not require polarization, new PXI modules were purchased. The reason for this was that, so called, Field Point Modules, currently used for target operation and control, will soon become obsolete. The new

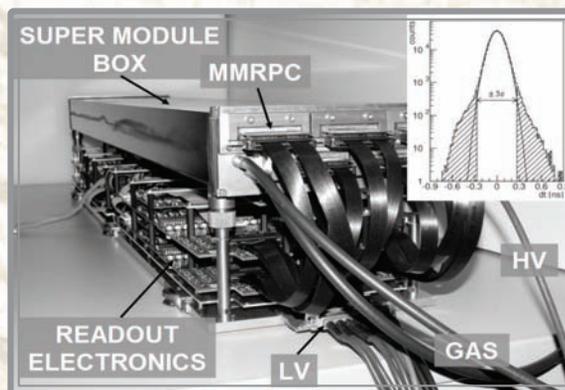


Figure 7. A single SM mounted with the read out electronics below. Inset in the right-up corner shows the resolution of the ToF spectrum of $\sigma_{ToF} < 88$ ps for fast pions. The non-Gaussian tails (hatched areas) outside the shown $\pm 3\sigma$ interval contain less than 0.6% of all particles.

modules are the NI PXI 2586 relay module and the NI PXI 8512 Control Area Network module. The first unit is used for switching applications and the second for control and communication of various remote signals.



Fig. 8: New Nuclear Instruments modules.

EDUCATION

Members of the Division have been involved in lecturing at the undergraduate and graduate level in 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. Four Ph. D. theses, one M.Sc. and one B.Sc. thesis were completed under the mentorship of division staff.



Fig. 9. Remotely operated vehicle (ROV) UNCROSS ready for testing of its maritime characteristics.

AWARDS

Igor Gašparić, Roman Čaplar, Suzana Szilner, Nada Horvatinčić, Milorad Korolija, Ivan Supek, Raul Horvat, Milica Krčmar, Milko Jakšić and Vuko Brigljević received awards from the RBI director for Scientific accomplishments in 2011. Tome Antičić was appointed by the Croatian Ministry of Science, Education, and Sports as expert for the FP7 Cooperation – Energy. Jadranka Barešić was awarded the Go8 fellowship (Coalition of leading Australian universities), Research School of Earth Sciences, ANU, Canberra, Australia, March 8 –August 15, 2011.

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 in investigation of karst environment and dating, Bogomil Obelić
10. Development and application of nuclear analytical methods, Jasmina Obhodaš
11. Development of the methods for illicit trafficking control, Dario Matika and Davorin Sudac
12. Hadronic physics between the experiments and QCD models, Alfred Švarc
13. Test of special relativity by the Ives-Stilwell type experiment, Saša Blagus

Research, developmental and international projects

1. FP7 project: “Particle Detectors”, Tome Antić project coordinator
2. 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)
3. Support of Public and Industrial Research using Ion beam Technology (SPIRIT), Milko Jakšić (EU FP7 project No. 227012)
4. Hadron Physics 2, Roman Čaplar, Ivan Supek, Alfred Švarc, Ivan Supek activity leader in SPINMAP subprogram (EC FP 7 programme contract 227431.
5. Underwater Coastal Sea Surveyor (UNCROSS), Jasmina Obhodaš (EU FP7-SEC-2007-1, Contract No. 218148.
6. Studies, training, socio-economical valorization and management of natural, cultural and monumental property for the promotion of the local societies of Latin America (Argentina, Brazil and Mexico, STRAVAL, FP7- PEOPLE Project, Bogomil Obelić
7. Network in solid waste and water treatment between Europe and Mediterranean countries (SOWAEUMED), FP7 - REGPOT Project, Bogomil Obelić
8. Research project Experimental nuclear physics inputs for thermonuclear runaway, prin-

- cipal investigator Neven Soić, part of the collaborative project Physics of compact objects: explosive nucleosynthesis and evolution, EuroGENESIS programme of the European Science Foundation
9. Physics of nuclei and hadrons at high energies, Roman Čaplar (International collaboration project RBI-KFKI Research Institute for Particle and Nuclear Physics, Budapest via Croatian (HAZU) and Hungarian Academy of Science)
 10. Protection of cultural and natural heritage using ^{14}C dating by AMS method, UNESCO project, Nada Horvatinčić
 11. Influence of climatic and environmental change on the processes of biologically induced calcite precipitation in Plitvice Lakes, Project with Plitvice National Park, Nada Horvatinčić
 12. Enhancement of Ion Beam Analysis Capabilities Using Novel Detection Systems for PIXE, RBS and STIM, IAEA CRP project No 15988, Stjepko Fazinić
 13. Using environmental isotopes for evaluation of streamwater/groundwater interactions in selected aquifers in the Danube basin, Project IAEA RER8016, Nada Horvatinčić
 14. Measurement of ^3H activity in natural waters with electrolytic enrichment, bilateral project Croatia - Slovenia, Jadranka Barešić (2010 – 2011), since 1.3.2011. Ines Krajcar Bronić
 15. ^{14}C and ^{137}Cs in sediments - comparison of methods and application to recent sediments, bilateral project Croatia – Serbia, Ines Krajcar Bronić
 16. OPERA collaboration, Ante Ljubičić (International collaboration between RBI, CERN (Switzerland) and LNGS (Gran Sasso, Italy))
 17. CERN Axion Solar Telescope (CAST) experiment, Milica Krčmar (International collaboration between RBI and CERN (Switzerland))
 18. ALICE collaboration, Anticic (International collaboration between RBI and CERN (Switzerland))
 19. NA61 collaboration, Kadija (International collaboration between RBI and CERN (Switzerland))
 20. NA49 collaboration, Susa (International collaboration between RBI and CERN (Switzerland))
 21. Pierre Auger observatory, Argentina
 22. Development of frozen spin polarized target for Crystal Ball Collaboration at MAMI, Ivan Supek (University of Mainz for EU program I3HP TNA Contract)

SELECTED INVITED LECTURES

1. Lakić B, Status and perspectives of the CAST experiment, 12th International Conference on Topics in Astroparticle and Underground Physics (TAUP), Munich, Germany, September 5-9, 2011
2. Jakšić M, Thin film solar cells - ion beams as a tool for characterization, radiation hardness tests and fabrication, Low-cost Solar Cells 2011: Opportunities and Challenges for Green Energy, Skopje, Macedonia, May 15-18, 2011.
3. Valković V, Inspection of the objects on the sea floor by using 14 MeV tagged neutrons, The Second International Conference on Advancements in Nuclear Instrumentation, Measurement Methods and their Applications (ANIMMA), Ghent, Belgium, June 06-09, 2011.
4. Švarc A, Amplitude Analysis in Hadron Spectroscopy, ECT* Trento, Italy, 24 - 28 January 2011.
5. Švarc A, Poles as a link between QCD and scattering theory (old and contemporary knowledge). Sixth International Workshop on Pion-Nucleon Partial-Wave Analysis and the Interpretation of Baryon Resonances, Washington DC, USA, 23–27 May 2011.
6. Ceci S, The extraction of resonance properties, Sixth International Workshop on Pion-Nucleon Partial-Wave Analysis and the Interpretation of Baryon Resonances, Washington DC, USA, 23–27 May, 2011,.
7. Basrak Z, Energy deposition in heavy-ion reactions at intermediate energies. Workshop on Clusters in Nuclei and Nuclear Matter, Trento, Italy, 13-17 June 2011.
8. Basrak Z, Nikola Cindro - scientist, teacher and man of culture. Highlights in Heavy-Ion Physics, Split, Croatia, 22-24 September 2011.
9. Basrak Z, Constancy of thermal energy in heavy ion collisions (in Croatian). 7th Sci-

entific meeting of Croatian Physical Society, Primošten, Croatia, 13-16 October 2011.

10. Soić N, Zagreb initiative on research in nuclear astrophysics. Highlights in Heavy-Ion Physics, Split, Croatia, 22-24 September 2011.
11. Szilner S, Quasi-elastic reactions: an interplay of reaction dynamics and nuclear structure. FUSION11, Saint Malo, France, 2-6 May 2011.
12. Szilner S, Properties of nuclear reactions around the Coulomb barrier (in Croatian). 7th Scientific meeting of Croatian Physical Society, Primošten, Croatia, 13-16 October 2011.
13. Brigljević V, Standard Model Measurements with CMS, Beyond the Standard Model: results with the 7 TeV LHC Collision Data, ICTP, Trieste (Italy), 19-23 September 2011.
14. Morović S, Measurement of WZ Production and search for WZ resonances with the CMS Detector, ICTP, Trieste (Italy), 19-23 September 2011.
15. Brigljević V, Introduction to LHC Physics, Sarajevo School of High Energy Physics, Sarajevo (Bosnia and Hercegovina), 11-14 May 2011.
16. Jakšić M: Review of nuclear microprobe applications in materials science, 13th International Conference on Nuclear Microprobe Technology and Applications, Lisbon, Portugal, July, 22-27, 2012.

SELECTED ORGANIZED CONFERENCES

1. 8th Symposium of Croatian Radiation Protection Association, Krk, Croatia, 13 – 15 April 2011, Bogomil Obelić and Ines Krajcar Bronić were members of the Scientific committee
2. Workshop/Case Study: Monitoring of water and lake sediment quality in natural environment, within FP 7 SOWAEUMED Project, organized at Plitvice Lakes, May 29 – June 1, 2011
3. International School of travertine and tufa, Abbadia San Salvatore (Siena), Italy, 5 – 9 September 2011, Nada Horvatinčić was a member of the Scientific committee.
4. 2nd Scientific meeting of Geology of Quar-

tar in Croatia, with international participation, Zagreb HAZU, March 25, 2011, Nada Horvatinčić was a member of organizing committee.

5. Highlights in Heavy-Ion Physics, Symposium in Honour of Nikola Cindro organized by RBI Laboratory for Nuclear Physics and Croatian Academy of Sciences and Arts, co-chaired by Suzana Szilner and Zoran Basrak, Split, Croatia, 22-24. September 2011. (Zoran Basrak; Roman Čaplar; Mladen Kiš, Miljanić, Đuro; and Suzana Szilner were members of the Organization Committee from RBI).
6. NA61/CERN Collaboration week at RBI. Organized by Tome Antičić, Krešo Kadija, Vlasios Petoussis, Tatjana Šuša.
7. DAQ workshop organized through the FP7 project Particle Detectors. Organized by Mladen Kiš, Tome Antičić, Milko Jakšić, Stjepko Fazinić.
8. Course on particle phenomenology “Introduction to Supersymmetry”, given by G. Senjanović and M. Nemevšek. Organized by Vuko Brigljević, RBI, 12-16 December 2011.

SELECTED PUBLICATIONS

1. Pastuović Ž, Vittone E, Capan I, Jakšić M. Probability of divacancy trap production in silicon diodes exposed to focused ion beam irradiation. *Appl Phys Lett* **98** (2011) 092101-1.
2. Fazinić S, Mandić L, Kavčić M, Božičević I. Crossover and valence band $K\beta$ X-rays of chromium oxides, *Spectrochimica Acta Part B* **66** (2011) 461.
3. Fazinić S, Mandić L, Kavčić M, Božičević I. Parametrization of $K\beta$ ” and $K_{\beta 2,5}$ X-ray contributions in $K\beta$ spectra of 3d transition metal compounds. *J Anal Atom Spectrom* **26** (2011) 2467.
4. Joulaeizadeh L et al. (BBS Collaboration-RBI: Gašparić I, Čaplar R). Pionic fusion in light-ion systems. *Phys Lett B* **694** (2011) 310.
5. Corradi L et al. (PRISMA Collaboration-RBI: Jelavić-Malenica D, Soić N, Szilner S). Single and pair neutron transfers at sub barrier energies. *Phys Rev C* **84** (2011) 034603.
6. Arik M. et al. (CAST Collaboration-RBI:

- Jakovčić, K, Krčmar M, Lakić B, Ljubičić A). Search for sub-eV mass solar axions by the CERN Axion Solar Telescope with ^3He buffer gas. *Phys Rev Lett* **107** (2011) 261302-1.
7. Horvat R, Kekez D, Krčmar M, Krečak Z, Ljubičić A. Hunting up low-mass bosons from the Sun using HPGe detector. *Phys Lett B* **699** (2011) 21.
 8. Horvat R, Trampetić J. Constraining noncommutative field theories with holography. *JHEP* **1101** (2011) 112.
 9. Horvat R. Holographic bounds and Higgs inflation. *Phys Lett B* **699** (2011) 174.
 10. Barešić J, Horvatinčić N, Roller-Lutz Z. Spatial and seasonal variations in the stable C isotope composition of dissolved inorganic carbon and in physico-chemical water parameters in the Plitvice Lakes system. *Isot Environ Health Stud* **47** (2011) 316.
 11. Ceci S, Döring M, Hanhart C, Krewald S, Meißner U, Švarc A. Relevance of complex branch points for partial wave analysis. *Phys Rev C* **84** (2011) 015205-1.
 12. Hadžimehmedović M, Ceci S, Švarc A, Osmanović H, Stahov J. Poles as the only true resonant-state signals extracted from a worldwide collection of partial wave amplitudes using only one, well controlled pole-extraction method. *Phys Rev C* **84** (2011) 035204-1.
 13. Osmanović H, Ceci S, Švarc A, Hadžimehmedović M, Stahov J. Stability of the Zagreb realization of the Carnegie-Mellon-Berkeley coupled-channels unitary model. *Phys Rev C* **84** (2011) 035205-1.
 14. Buljan M, Bogdanović-Radović I, Karlušić M, Desnica U, Radić, N, Jakšić M, Salamon K, Dražić G, Bernstorff S, Holý V. Design of quantum dot lattices in amorphous matrices by ion beam irradiation. *Phys Rev B* **84** (2011) 155312.
 15. Montanari D et al. (PRISMA-CLARA Collaboration-RBI: Szilner S). Probing the nature of particle-core couplings in ^{49}Ca with γ spectroscopy and heavy-ion transfer reactions. *Phys Lett B* **697** (2011) 288.
 16. Szilner S et al. (PRISMA Collaboration-RBI: Jelavić-Malenica D, Soić N). Interplay between single-particle and collective excitations in argon isotopes populated by transfer reactions. *Phys Rev C* **84** (2011) 014325.
 17. Berghauser H for Crystal Ball Collaboration (RBI: Knežević A, Korolija M, Mekterović D, Mićanović S, Supek I, Zamboni I). Determination of the eta-transition form factor in the gamma $p \rightarrow p \eta \rightarrow p \gamma e^+ e^-$ reaction. *Phys Lett B* **701** (2011) 562.
 18. Chatrchyan S et al. (CMS Collaboration-RBI: Brigljević V, Đurić S, Kadija K, Morović S). Measurement of the Inclusive W and Z Production Cross Sections in pp Collisions at $\sqrt{s} = 7$ TeV with the CMS experiment. *J High Energy Phys* **10** (2011) 132.
 19. Chatrchyan S et al. (CMS Collaboration-RBI: Brigljević V, Đurić S, Kadija K, Morović S). Measurement of W_{gamma} and Z_{gamma} production in pp collisions at $\sqrt{s} = 7$ TeV. *Phys Lett B* **701** (2011) 535.
 20. Kiš M et al. (FOPI Collaboration). A Multi-strip Multi-gap RPC Barrel for Time-of-Flight Measurements. *Nucl Instr and Meth A* **646** (2011) 27.

Book chapter

1. Obhodaš J, Valković V: Heavy Metals in Coastal Sea Sediments of the Eastern Adriatic Sea, in Heavy Metal Sediments, Lucia A. Sanz (ed.), Nova Science Publishers, New York, 2011. pp 35-58.

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 primary mission of the Division of Materials Physics is the acquisition and accumulation of new knowledge through frontier research in the fundamental natural sciences - physics, chemistry and interdisciplinary research. We aim to contribute to the development of the Republic of Croatia as a knowledge-based society embedded in the wider European scientific community. We are focused on fundamental and applied studies of the physical parameters and processes which describe and connect the microscopic, mesoscopic and macroscopic properties of condensed matter and molecules. Nanoscience and nanotechnology has been the most active direction in terms of both fundamental scientific research and technology development. Fundamental research in the field of molecular and solid state physics placed special emphasis on vibrational spectroscopy in a wide range of

systems, while strongly nonlinear effects in laser-matter interaction, and self-organization in condensed systems continued to be subjects of intensive research.

TOP ACHIEVEMENTS

Bi-doped goethite-hematite nanostructures and their catalytic activity in the degradation of an actual pesticide

Tailoring the iron-based catalysts' morphology through the addition of Bi to the structure resulted in catalytic activity related to the crystal phases and morphology of the catalysts. It was found that a homogenous mixture of hematite and BiFeO_3 nanoparticles exhibits the best performance. The catalysts were stable in terms of metal leaching under the conditions employed (Fig.1), while hydroxyl radicals seem to be produced at the catalyst surface (Gajović et al., 2011).

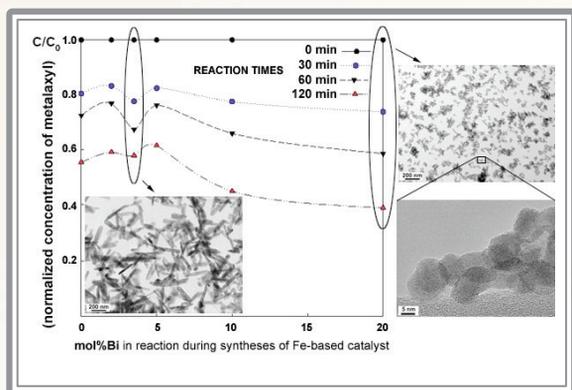


Fig. 1. Normalized concentration of metalaxyl at different reaction times in photo-Fenton-like experiments as a function of the mol% of bismuth in samples prepared by hydrothermal treatment after separate precipitation of the starting solutions of iron salts and bismuth salt and TEM images of samples with 3.5 mol% Bi and 20 mol% Bi (best performance)

Populations of the three major backbone conformations in 19 amino acid dipeptides

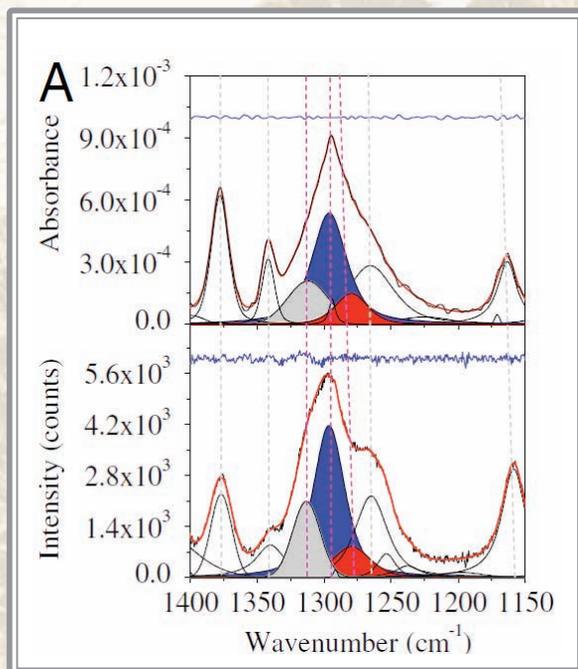


Fig. 2. ATR infrared (upper) and Raman spectra of glycine water solution with molar ratio 0.01. Grey band corresponds to PII, blue band to α_R , while red band corresponds to β conformation.

Vibrational spectroscopy was used for determination of the relative percentage of polyprolyne P_{II}, and two other - α_R and β conformations - in water solutions of dipeptides, by fitting of observed intensities with calculated bands in the 1270 - 1320 cm^{-1} interval. The ratio of P_{II} i β populations was taken from the $^3J(\text{H}_N, \text{H}\alpha)$ constants obtained with NMR spectroscopy. Equipotential energy surface is drastically altered in water solutions, becomes shallow and the minima broad. Raman spectroscopy proved to be a valuable method to probe the surface in these circumstances (Grdadolnik et al., 2011).

Correlation between short ordered fractal structures at the molecular level and macroscopic quantity enables detection of a second order phase transition

A strong correlation between the fractal dimension and the corresponding compressibility modulus of different amphiphilic materials has been found. It allows unambiguous identification of the onset of percolation – a second order phase transition that is otherwise difficult to detect. The proposed method should facilitate a more efficient application of the percolation theory in the further study of processes and structures at an interface during compression (Risović et al., 2011).

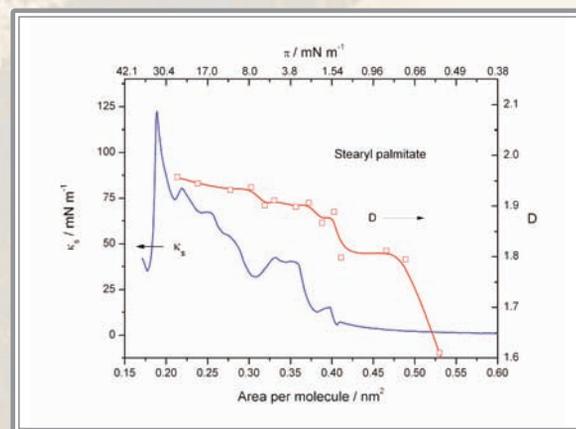


Fig. 3. The compressibility modulus and fractal dimension of the stearyl- palmitate monolayer vs. A. The correlation coefficient between κ_s vs. D is $R = 0.859$.

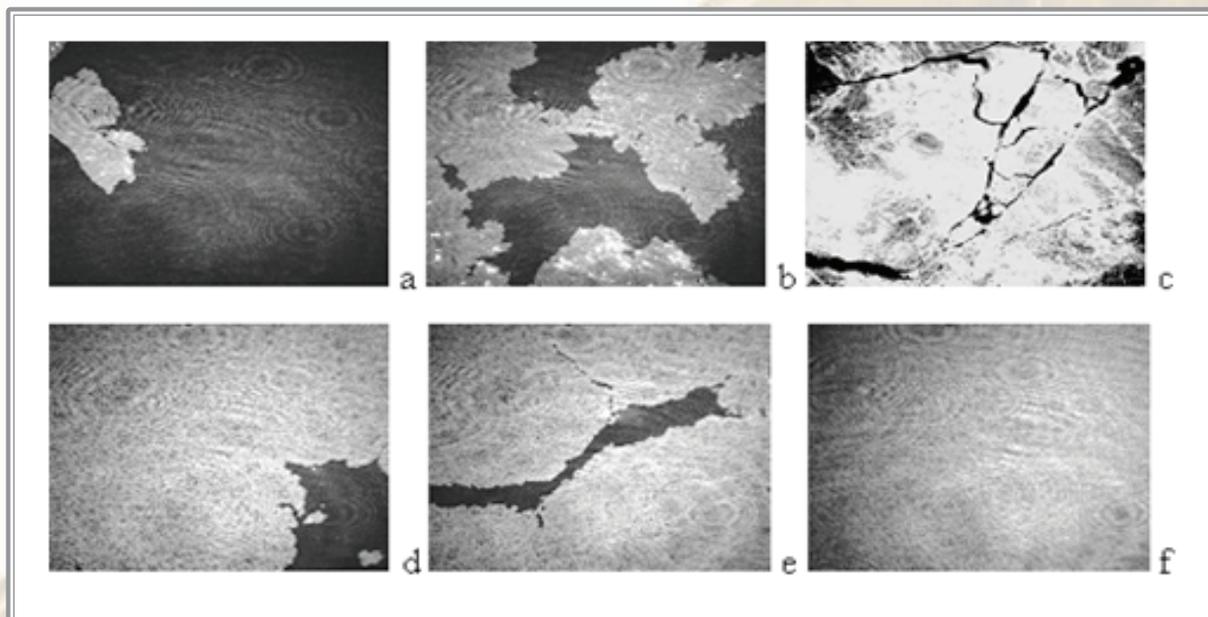


Fig. 4. Compression of the stearyl palmitate monolayer. BAM images of the monolayer structures at a) 0.3 mN m⁻¹, b) 0.6 mN m⁻¹, c) 1.2 mN m⁻¹ (just before percolation), d) 1.7 mN m⁻¹ (after percolation), e) 3.5 mN m⁻¹, f) 7.8 mN m⁻¹.

Microwave-Assisted Nonaqueous Sol-Gel Chemistry for Highly Concentrated ZnO-Based Magnetic Semiconductor Nanocrystals

Various transition metal (TM) doped zinc oxide nanoparticles with the composition TM_(x)Zn_(1-x)O (TM = V, Mn, Fe, Co, and Ni; x = 0.01-0.3) were prepared by a microwave-assisted nonaqueous sol-gel route in benzyl alcohol within a few minutes. The high doping levels in the range of 20-30 atom % achieved for Co and Fe provide a promising opportunity to study the magnetic properties of such potential diluted magnetic semiconductors (Bilecka et al., 2011).

Ionic-Liquid Synthesis Route of TiO₂(B) Nanoparticles for Functionalized Materials

A fast and soft ionic-liquid synthesis route is presented to obtain monophasic TiO₂(B) nanoparticles. The material presents interesting electrochemical properties when used as the negative electrode (charge capacity, re-

versibility, stability, and low temperature performance) in Li batteries (Wessel et al., 2011).

EFG silicon for low-cost solar cells

The successful application of a capacitance transient technique in the study of extended defects (dislocations and grain boundaries) was observed in EFG silicon for use in low-cost solar-cells (Slunjski et al., 2011).

Ion implantation induced defects

We developed the successful separation and analysis of interstitial and vacancy-related defects in n-type silicon single crystals implanted with silicon MeV ions (Pastuović et al., 2011).

Design of quantum dot lattices by ion beam irradiation

A highly controllable self-assembly of semiconductor quantum dots and metallic nanoparticles in a solid amorphous matrix, induced by ion beam irradiation of an amor-

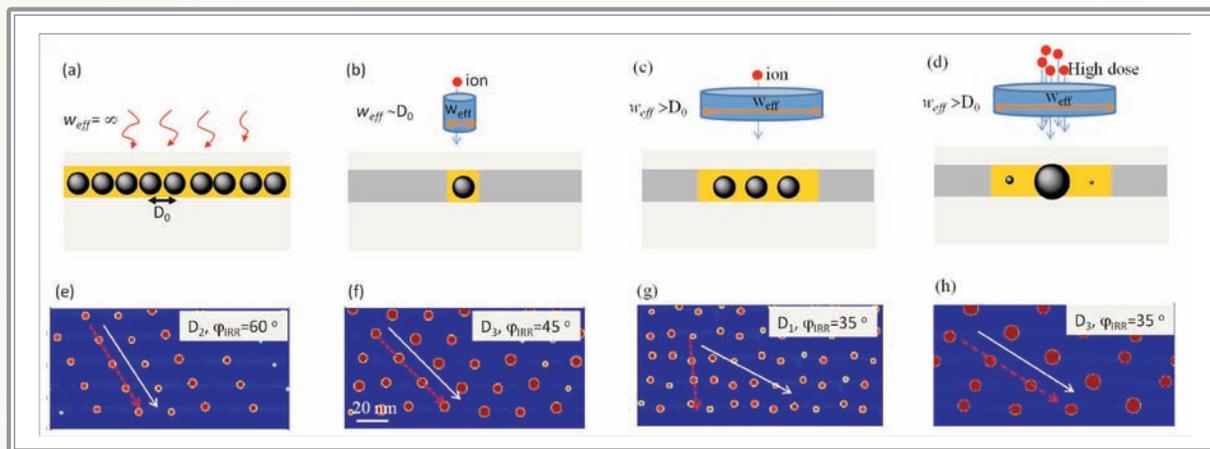


Fig. 5. (a) Standard thermal annealing. The intrinsic separation of the QDs is L_0 . (b) Effect of a single ion when the width of its track is comparable to L_0 . A nucleation of a single QD within the track volume is possible. (c) Irradiation by a single ion if the ion track is broader than L_0 ; several QDs with the mean separation of L_0 can be created in the irradiated volume. (d) Influence of a high irradiation dose; the Ostwald ripening process takes place.

phous multilayer was demonstrated. We have shown experimentally and theoretically the possibility to tune the basic structural properties of the quantum dots over a wide range (Buljan et al., 2011).

EDUCATION

Members of the Division of Materials Physics were involved in teaching of 10 undergraduate and 4 postgraduate courses of physics and related topics at the Faculty of Sciences, Faculty of Electrical Engineering and Computing, Faculty of Chemical Engineering and Technology in Zagreb and elsewhere.

AWARDS

Igor Djerdj, Vlasta Mohaček-Grošev, Maja Buljan and Nikola Radić received the annual RBI Director's Award for excellence in science and publishing in highly rated scientific journals. Davor Ristić received the annual RBI Director's Award for winning a competitive grant with funding of more than 70.000 EUR. Jasminka Popović received an award for originality, scientific content and presentation of the poster entitled "Structure and

microstructure of Sn-doped indium oxide" at the 44th Course of the International School of Crystallography: The Power of Powder Diffraction, Erice, Italy, June 02-12, 2011. Novice Martina Vrankić received an award for originality, scientific content and presentation of the poster entitled "Structural study of nanocrystalline Ti-doped gahnite" at the 44th Course of the International School of Crystallography: The Power of Powder Diffraction, Erice, Italy, June 02-12, 2011.

Research program supported by the Ministry of Science, Education and Sports

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

Research 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

Research, developmental and international projects

1. Influence of quantum confinement on vibrational properties in nanocrystalline silicon, Davor Gracin (Croatian-Slovenian bilateral project)
2. Nanocrystalline silicon as a possible candidate for "third generation" of solar cells, Davor Gracin (Croatian-Slovenian bilateral project)
3. Laser-induced surface self-organization: formation of surfaces with special properties, Stjepan Lugomer (Croatia-Hungary)
4. Study of oxygen precipitation and structural defects in single crystal silicon, Branko Pivac (Croatian - Chinese Scientific and Technological Cooperation)
5. Silicon nanocrystals solar cells ... Properties and characterization, Ivana Capan (Unity Through Knowledge Fund – Young Researchers Program; October 1st 2009 – September 30th 2011)
6. The origin of structural defects in silicate glasses and their effects upon the properties, Davor Gracin (National Science Foundation of Croatia)

SELECTED INVITED LECTURES

1. Gajović A, Šantić A, Krsmanović R, Silva AMT, Su D, Čeh M. Microscopy in analysis of functional ceramics and nanostructures. Proceedings 10th Multinational Congress on Microscopy 2011, Urbino, September 4-9, 2011.

2. Radić N, Dubček P, Maksimović A, Salamon K, Jerčinović M, Dražić G, Bernstorff S. A growth of C/W multilayers – Experiment & Modelling. 15th International Conference on Thin Films, Kyoto, Japan, November 08-11, 2011.

SELECTED PUBLICATIONS

1. Bilecka I, Luo L, Djerdj I, Rossell MD, Jagodić M, Jagličić Z, Masubuchi Y, Kikkawa S, Niederberger M. Microwave-Assisted Nonaqueous Sol-Gel Chemistry for Highly Concentrated ZnO-Based Magnetic Semiconductor Nanocrystals. *J Phys Chem C* **115** (2011) 1484.
2. Buljan M, Bogdanović-Radović I, Karlušić M, Desnica U, Radić N, Jakšić M, Salamon K, Dražić G, Bernstorff S, Holy V. Design of quantum dot lattices in amorphous matrices by ion beam irradiation. *Phys Rev B* **84** (2011) 155312-1.
3. Gajović A, Silva AMT, Segundo RA, Šturm S, Jančar B, Čeh M. Tailoring the phase composition and morphology of Bi-doped goethite-hematite nanostructures and their catalytic activity in the degradation of an actual pesticide using a photo-Fenton-like process. *Appl Catal B - Environ* **103** (2011) 351.
4. Grdadolnik J, Mohaček Grošev V, Baldwin R, Avbelj F. Populations of the Three Major Backbone Conformations in 19 Amino-Acid Dipeptides. *Proc Natl Acad Sci USA* **108** (2011) 1794.
5. Meljanac S, Meljanac D, Samsarov A, Stojić M. Kappa Snyder deformations of Minkowski spacetime, realizations, and Hopf algebra. *Phys Rev D* **83** (2011) 065009-1.
6. Pastuović Ž, Vittone E, Capan I, Jakšić M. Probability of divacancy trap production in silicon diodes exposed to focused ion beam irradiation. *Appl Phys Lett* **98** (2011) 092101-1.
7. Risović D, Frka S, Kozarac Z. Application of Brewster angle microscopy and fractal analysis in investigations of compressibility of Langmuir monolayers. *J Chem Phys* **134** (2011) 024701.

8. Slunjski R, Capan I, Pivac B, Le Donne A, Binetti S. Effects of low-temperature annealing on polycrystalline silicon for solar cells. *Sol Energy Mater Sol Cells* **95** (2011) 559.
9. Stepanić V, Koštrun S, Malnar I, Hlevnjak M, Butković K, Čaleta I, Dukši M, Kragol G, Makaruha-Stegić O, Mikac L, Ralić J, Tatić I, Tavčar B, Valko K, Zulfikari S, Munić V. Modeling Cellular Pharmacokinetics of 14- and 15-membered Macrolides with Physicochemical Properties. *J Med Chem* **54** (2011) 719.
10. Sović D, Gajović A, Iveković D. Bioelectrocatalytic and biosensing properties of horseradish peroxidase covalently immobilized on (3-aminopropyl)trimethoxysilane-modified titanate nanotubes. *Electrochim Acta* **56** (2011) 9953.
11. Wessel C, Zhao L, Urban S, Ostermann R, Djerdj I, Smarsly B, Chen L, Hu Y-S, Sallard S. Soft and fast ionic liquid synthesis route of TiO₂(B) nanoparticles for functionalized materials. *Chem-Eur J* **17** (2011) 775.

Division of Laser and Atomic Research and Development

<http://www.irb.hr/en/zlair>

LAIR

DIVISIONAL ORGANIZATION

Head: Hrvoje Zorc

The Division of Laser and Atomic R&D (Zavod za laserska i atomska istraživanja i razvoj) consists of the following laboratories:

- ⇒ Laboratory of Thin Films and Optics, Vesna Janicki
- ⇒ Multipurpose workshops, Eduard Švegel



tion, nonlinear decomposition of multichannel medical images with application in contrast enhancement of multi-phase CT image and multispectral images in pathology, an independent component analysis based approach to dictionary learning for efficient representation of images of natural scenes with applications in filling-in missing values, denoising of images corrupted by salt and pepper noise and consensus-based regression with applications in the prediction of anti-tumor activity of virtual chemical compounds.

The Division has also developed a strategic project in the field of national security, together with an industrial partner and in coordination with the Ministry of Defence.

OVERVIEW OF THE DIVISION

The mission of the Division is to expand and strengthen our knowledge in the fields of imaging and non-imaging optics, photonics and the fundamentals of optical thin films. In addition, we aim to develop the application of these basic disciplines in the field of national security.

The Division is currently developing several strategic projects. These include modelling of thin film mixtures using effective medium theories, research on the plasmonic properties of metallic nanoclusters, use of plasmonic materials in optical multilayer design, characterization and modelling of very thin metallic layers, sparse component analysis and a tensor factorization approach to feature extraction from multispectral images and protein and/or gene expression levels with applications in disease (cancer) diagnosis and biomarker identifica-

TOP ACHIEVEMENTS

Near-field coupling of metal nanoparticles under tightly focused illumination

The influence of strongly focused radiation on the electromagnetic interaction of metal particles was studied. The near-field distribution of silver dimers was calculated by com-

binning a multiple scattering approach and the multipolar expansion of focused beams based on the Richards–Wolf description of diffracting systems. These results show that tight focusing can induce larger maximum field enhancement and stronger localization of the near field than can plane wave illumination. Additional plasmonic resonances can be obtained due to the presence of different polarization contributions at focus (Sancho-Parramon et al., 2011).

Design and production of bicolour reflecting coatings with Au metal island films

The optical properties of metal island films (MIFs) can be combined with interference of dielectric coatings. A set of multi-layer designs containing metal clusters reflecting different colours from the front and back side of a coating was obtained by numerical optimization. The chosen designs, representing a range of feasible colours, were deposited by electron beam evaporation. Spectrophotometric and ellipsometric measurements verified that the produced coatings exhibited optical performance in excellent agreement with that calculated from designs. Numerical optimization was verified as a useful method in the design of coatings containing MIFs. This approach will ease the implementation of metal clusters into multilayer designs and broaden the applications of MIFs (Janicki et al., 2011).

A methodology for contrast-enhanced unsupervised segmentation of multi-spectral (color) microscope image

A methodology has been proposed for contrast-enhanced unsupervised segmentation of a multi-spectral (color) microscope image of a principally unstained specimen (Kopriva et al., 2011). The methodology exploits spectral diversity and spatial scarcity to find anatomical differences between ma-

terials (cells, nuclei and background) present in the image. The methodology was validated on experimental multi-spectral microscope images of unstained nerve fibers (n. ischiadicus) and unstained white pulp in spleen tissue. The methodology can be used for additional contrast enhancement with stained specimen images.

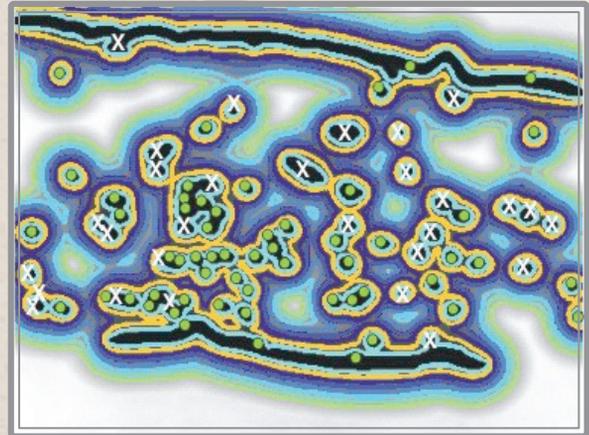


Fig. 1. Isolines of nonlinearly segmented image of unstained specimen of sciatic nerve fibers (nervus ischiadicus). False positive spots are marked by white crosses.

EDUCATION

Division members teach at the Faculty of Science, University of Zagreb, University of Applied Sciences Velika Gorica, and Faculty of Electrical Engineering and Computing, University of Zagreb.

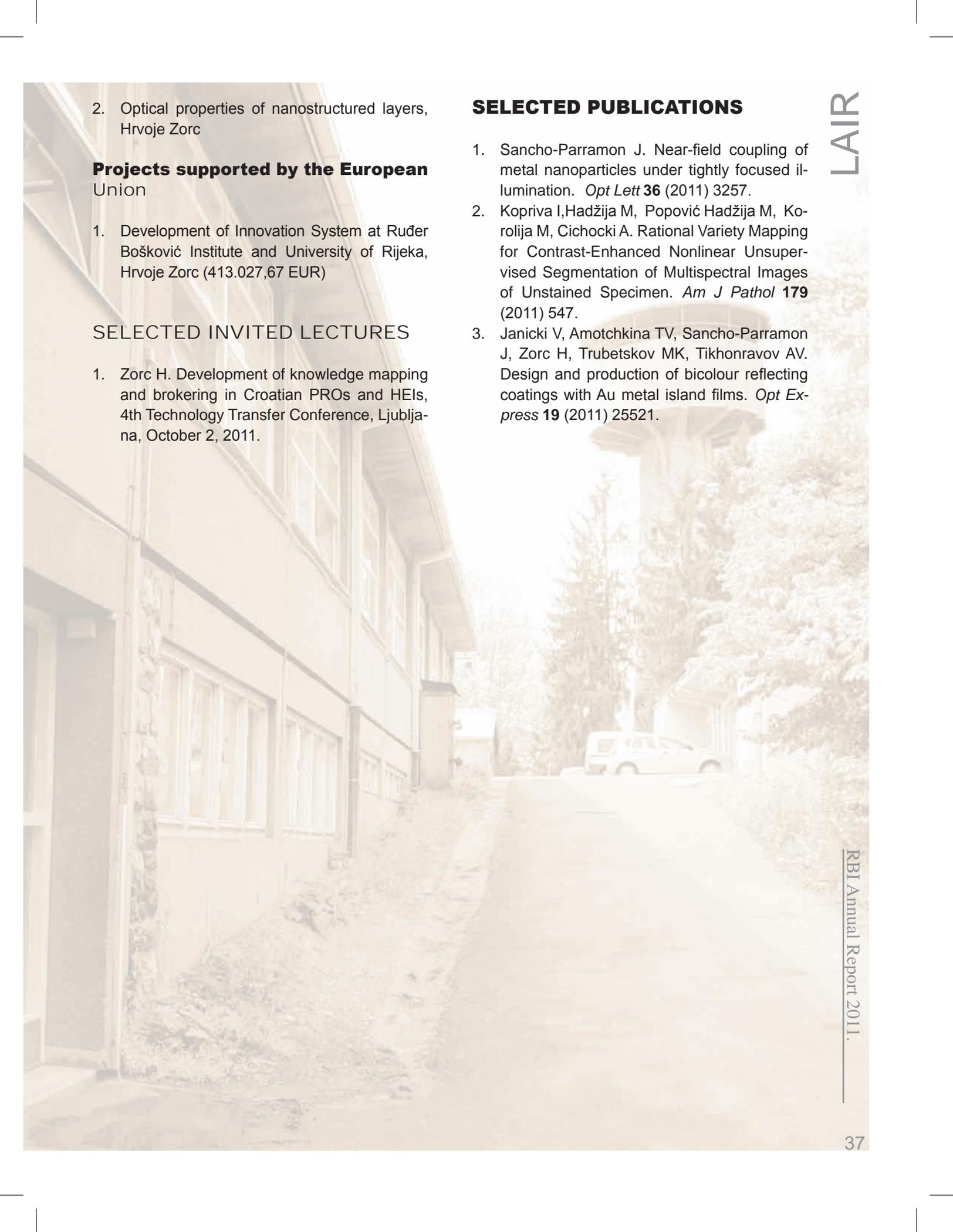
AWARDS

Award to Ivica Kopriva: The Annual award of the RBI Director for a high quality research article in *The American Journal of Pathology*.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Analysis of multispectral data, Ivica Kopriva

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- The background of the page is a faded, sepia-toned photograph of a long, multi-story building with a series of windows on the left side. A paved road or driveway runs alongside the building, leading towards a large, modern, cylindrical structure in the distance, possibly a water tower or a monument. The overall scene is bright and somewhat washed out.
2. Optical properties of nanostructured layers, Hrvoje Zorc

Projects supported by the European Union

1. Development of Innovation System at Ruđer Bošković Institute and University of Rijeka, Hrvoje Zorc (413.027,67 EUR)

SELECTED INVITED LECTURES

1. Zorc H. Development of knowledge mapping and brokering in Croatian PROs and HEIs, 4th Technology Transfer Conference, Ljubljana, October 2, 2011.

SELECTED PUBLICATIONS

1. Sancho-Parramon J. Near-field coupling of metal nanoparticles under tightly focused illumination. *Opt Lett* **36** (2011) 3257.
2. Kopriva I, Hadžija M, Popović Hadžija M, Korolija M, Cichočki A. Rational Variety Mapping for Contrast-Enhanced Nonlinear Unsupervised Segmentation of Multispectral Images of Unstained Specimen. *Am J Pathol* **179** (2011) 547.
3. Janicki V, Amotchkina TV, Sancho-Parramon J, Zorc H, Trubetskov MK, Tikhonravov AV. Design and production of bicolour reflecting coatings with Au metal island films. *Opt Express* **19** (2011) 25521.

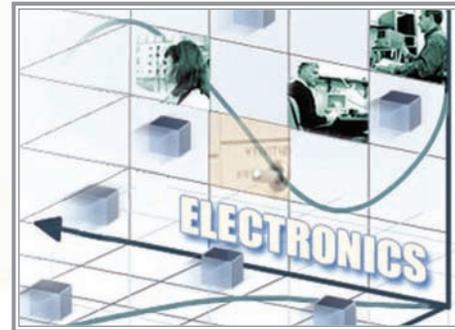


DIVISIONAL ORGANIZATION

Head: Tomislav Šmuc

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

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



TOP ACHIEVEMENTS

Knowledge technologies and computer science

REVIGO WEB service

A bioinformatics web server "REVIGO" was developed, targeting researchers that deal with Gene Ontology (GO) categories in

OVERVIEW OF THE DIVISION

The mission of the Division of Electronics is the development of techniques and approaches capable of tackling data and information overload, a common problem for most scientific disciplines and contemporary technology environments. Our techniques and approaches encompass a blend of signal processing and machine learning data mining, with modern programming paradigms, knowledge acquisition and representation technologies. The main application disciplines include biomedical engineering, biology (genomics/proteomics), and intelligent instrumentation and process modeling. The Division has 15 staff members, of which six are PhD students.

The members of the Division are involved in lecturing at the undergraduate, graduate and doctoral level at the Faculty of Electrical Engineering and Computing, the Faculty of Sciences as well as the School of Medicine at the University of Zagreb.



Fig. 1. Visualization of gene enrichment results within REVIGO WEB-service.

biology and biomedicine and providing a tool to describe and interpret their results (see Fig. 1). The lists of GO categories tend to be long and unintelligible; REVIGO can shorten them by eliminating redundant results and visualizing the rest in interactive plots based on GO semantic similarity measures. REVIGO had more than 1000 visitors from various countries in a single month. REVIGO was developed through an information technology grant (iProjekt) of the Ministry of Science, Education and Sport (MSES) (Supek et al., 2011).

ECML-PKDD 2011 Discovery Challenge

As part of the e-LICO project, Division members organized the „VideoLectures.Net Recommender System Challenge“ data mining competition in 2011. As the official challenge at ECML-PKDD 2011, one of the most high-profile conferences in the field of computer science, the challenge ran from April till July 2011 and attracted more than 60 active research teams from around the world. As part of the conference program, members of the Division of electronics also led the organization of the „Discovery Challenge Workshop“.

Object-oriented software library used for the development of algorithms and data experiments

We presented an object-oriented software library used for the development of algorithms, such as the LZ-trie structure for compressing static dictionaries and for data experiments. The developed software library is written in C++, and contains data structures, algorithms, and supporting functionality such as serialization. The functionality code consists of 87 classes and cc 9500 lines of code. The test code consists of cc 50 classes and approximately 5600 lines of code. The code is completely covered with unit tests. The software was developed using object oriented techniques, generic programming and

design patterns. It is used as a framework for algorithm development and experiments with data. After completion of the new algorithms currently under development, they will be published and the code will be made public under an open source license.

Start of the FOC project

In 2011 the Divisions of Electronics and Theoretical Physics started to work on the FP7 project: Forecasting Financial Crisis (FOC). FOC is a Scientific Project Financed by the FET OPEN Scheme in the field of Information and Communication Technology by the European Commission. The main research topic of the project is related to understanding and forecasting systemic risk and global financial instabilities. The project aims to offer a theoretical framework to measure systemic risk in the global financial market and financial networks, and deliver an ICT collaborative platform for monitoring systemic fragility and the propagation of financial distress across institutions and markets around the world. Experts will be able to evaluate algorithms and models to forecast financial crises as well as interactively visualize possible future scenarios.

Advanced signal processing techniques and measurement systems

Modeling systems with error/complexity constraints

A new Compound squared relative Error (CE) measure is proposed for meta-modeling complex systems and procedures with error and complexity constraints. Compared to other metrics, the proposed measure forces self-organization of polynomial neural networks by preferring the models having the smallest compound deviation in both accuracy and complexity from given thresholds and thus leads to more favorable models with respect to both constraints. Compared to a referent physical

model, the complexity (execution time) of the surrogate model can be decreased significantly with a corresponding degradation of its accuracy. The error/complexity characteristics of the model (Fig. 2) can be tuned by varying the thresholds and the weighting coefficient of the proposed measure (Marić et al., 2011).

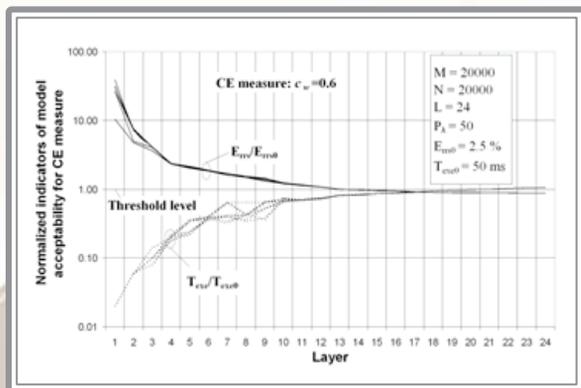


Fig. 2. Compound squared relative Error (CE) measure vs. model complexity for polynomial network model.

Implementation Framework for Artificial Neural Networks on FPGA

We proposed and are now developing a new framework for rapid deployment of a multilayer perceptron (MLP) type of Artificial neural network (ANN) on field programmable gate array (FPGA) platforms. The framework defines the internal architecture of the ANN implementation, and provides a means of automatic generation of a synthesizable VHDL-language for a digital hardware description-model of the ANN. The framework exploits several types of parallelism inherent to MLP which allows rapid evaluation of the network. The proposed framework has been evaluated on an ANN developed for a fall detector that recognizes a person fall event from real-time video stream, and it has been found to effectively speed up deployment of ANNs. The framework is currently being optimized to enable tuning of parallelism in the generated VHDL model of the network (Škoda et al., 2011).

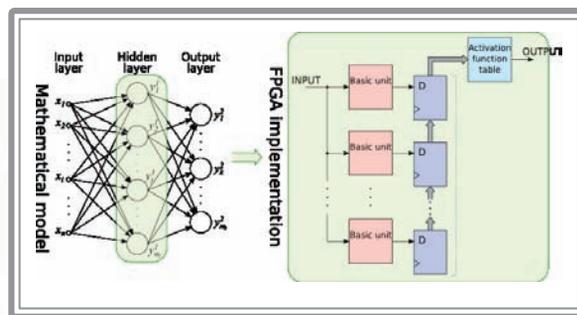


Fig. 3. LISSP develops new framework for rapid deployment of multilayer perceptron (MLP) type of artificial neural networks (ANN) on field programmable gate arrays (FPGA) platforms.

EDUCATION

In 2011, the members of the Division were involved in lecturing at the undergraduate, graduate and doctoral level at Faculty of Electrical Engineering and Computing („Algorithms and Data Structures“, S. Ristov), the Faculty of Sciences („Machine Learning“, T. Šmuc) and School of Medicine of the University of Zagreb („Knowledge Discovery“, D. Gamberger). Our PhD students were involved in organization of the International Science Summer School S3 for talented grammar school students, traditionally held in Višnja, Croatia.

Projects supported by the Ministry of Science, Education and Sport

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

Research, developmental and international projects

1. e-LICO: An e-Laboratory for Interdisciplinary Collaborative Research in Data Mining and Data-Intensive Science (EU-FP7 Collaborative Project), Tomislav Šmuc, Dragan Gamberger

2. FOC - Forecasting Financial Crises (EU-FP7 FET Project), Tomislav Šmuc, Dragan Gamberger
3. Reconfigurable embedded systems based assistive applications for elderly people (Croatian-Hungarian Intergovernmental S&T Programme), Branka Medved Rogina
4. Inductive Rule Learning (Croatian-Slovenian Intergovernmental S&T Programme), Dragan Gamberger
5. The Emergence of Southern Multinationals and their Impact on Europe (COST IS0905 action), Dragan Gamberger
4. Jović A, Gamberger D, Krstačić G. Heart Failure Ontology. *Bio-Alg Med-Sys* **7(2)** (2011) 101.
5. Smole Z, Nikolic N, Supek F, Šmuc T, Sbalzarini I, Krisko A. Proteome sequence features carry signatures of the environmental niche of prokaryotes. *BMC Evol Bio* **11** (2011) 26.
6. Antulov-Fantulin N, Bošnjak M, Žnidaršič M, Grčar M, Morzy M, Šmuc T. ECML/PKDD 2011 Discovery Challenge Overview. *Proc ECML-PKDD 2011 Discovery Challenge Workshop*, Antulov-Fantulin N, Morzy M, Smuc T (ed). Athens (2011) 7.

SELECTED PUBLICATIONS

1. Marić I, Ivek I. Self-Organizing Polynomial Networks for Time-Constrained Applications. *IEEE T Ind Electron* **58** (2011) 2019.
2. Supek F, Bošnjak M, Škunca N, Šmuc T. REVIGO summarizes and visualizes long lists of Gene Ontology terms. *PLoS One* **6(7)** (2011) e21800.
3. Škoda P, Lipić T, Srp Á, Medved Rogina B, Skala K, Vajda F. Implementation Framework for Artificial Neural Networks on FPGA. *Proc Vol. I. MEET&GVS 34rd International Convention MIPRO 2011*. Biljanović P, Skala K (ed). Zagreb: Croatian Society for Information and Communication Technology, Electronics and Microelectronics - MIPRO, 2011.

Chapters in the books

1. Supek F, Šmuc T. Distance Measures and Machine Learning Approaches for Codon Usage Analyses. In: *Codon Evolution - Mechanisms and Models*. Cannarozzi G, Schneider A (ed). Oxford: Oxford University Press, 2011. pp 229-244.

SELECTED ORGANIZED CONFERENCES

1. ECML-PKDD 2011 Discovery Challenge Workshop, Athens, Greece, 5.9.2011.

DIVISIONAL ORGANIZATION

Head: Aleksandar Sabljic

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

- ⇒ Laboratory for Chemical Kinetics and Atmospheric Chemistry, Branka Kovač
- ⇒ Theoretical Chemistry Group, Slobodan Bosanac
- ⇒ Laboratory of Chemical and Biological Crystallography, Marija Luić
- ⇒ Laboratory for Magnetic Resonances, Boris Rakvin
- ⇒ Laboratory for Synthesis and Processes of Selfassembling of Organic Molecules, Ivan Habuš



OVERVIEW OF THE DIVISION

The mission of the Division of Physical Chemistry is the discovery, exploitation, and dissemination of fundamental knowledge in the fields of protein science, coordination chemistry, spectroscopy, and computational and theoretical chemistry. Our aim is to become an internationally recognized Center of Excellence in selected areas of molecular research.

In 2011, members of the Division published more than 50 scientific papers in atmospher-

ic chemistry, chemical kinetics, structural chemistry, theoretical chemistry, modeling of physical and chemical processes, peptides and proteins research, and in other areas of biosciences. A significant number of articles were published in high ranking international journals such as: Chemical Communications, Inorganic Chemistry, Langmuir, Physical Chemistry Chemical Physics, Journal of Physical Chemistry A, Journal of Chemical Physics, Journal of Organic Chemistry, CrystEngComm, and Journal of the American Society for Mass Spectrometry. Half of these contributions were the result of domestic and international collaborations. A number of fruitful international collaborations demonstrate a strong presence of the Division in the European Research Area. As well, Division members contributed extensively (about 30 courses) to undergraduate and graduate education in Croatia.

Ligand exchange reactions at organopalladium compounds in the solid-state

Ball-milling of dipalladated azobenzenes with triphenylphosphine resulted in thermodynamically favourable bridged complexes. The formation of such products under these mechanochemical conditions is surprising since it requires highly complex changes in molecular structure during the reaction. These results will contribute to a better understanding of the structural transformations occurring during the mechanical processing of solid reactants and will have significant implications for the future design and synthesis of next generation coordination compounds (Cinčić et al., 2011).

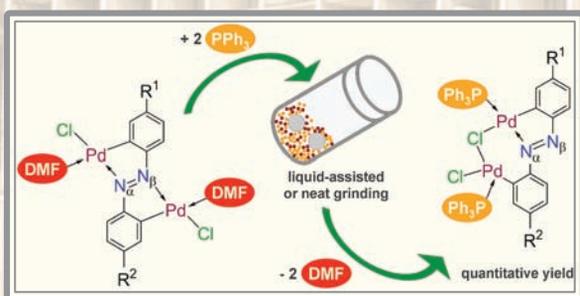


Fig. 1. Solid-state reactions of dipalladated azobenzenes with triphenylphosphine.

Fluxionality of Hydrogen Ligands in $\text{Fe}(\text{H})_2(\text{H}_2)(\text{PEtPh}_2)_3$

Extensive computational investigations along with quasielastic neutron scattering data were used to obtain a consistent picture of the extensive fluxionality of hydride and dihydrogen ligands in $\text{Fe}(\text{H})_2(\text{H}_2)(\text{PEtPh}_2)_3$ over a wide range of temperatures. Above 225 K we have identified a dynamical process with an activation energy of 0.44 kcal/mol which was attributed to a quantum dynamical exchange of dihydrogen and hydride ligands. Dynamics of this type may be important in hydrogen spillover from metal particles, and therefore need to be further elucidated in an effort to utilize this phenomenon (Došlić et al., 2011).

Polymorphism and Mesomorphism of Oligomeric Surfactants: Effect of the Degree of Oligomerization

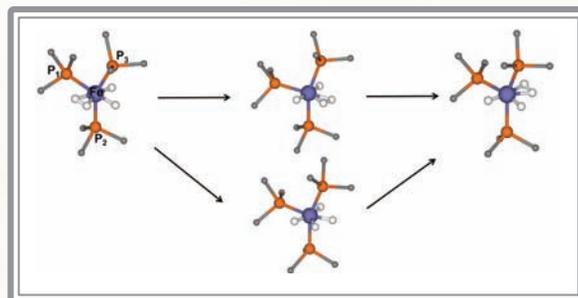


Fig. 2. High level theoretical analysis of the iron complex provides a good account of its structural and energetic properties, including dihydrogen rotation and dihydrogen-hydride exchange.

In spite of numerous papers dealing with the solution and interfacial properties of oligomeric surfactants, there are relatively few reports on the structural and thermal behavior of the first member in a series of dimeric surfactants. The results presented in this paper give new insight into the structural and amphotropic properties of oligomeric surfactants, i.e. quaternary dodecyldimethylammonium ions with two, three or four chains connected by an ethylene spacer at the head group level (Jurašin et al., 2011).

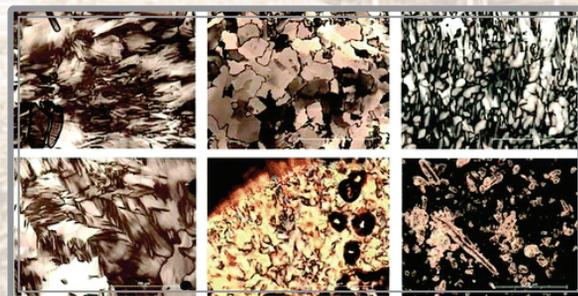


Fig. 3. Textures obtained from polarizing microscopy for hydrated trimer (the first row) and tetramer (the second row) during a heating and cooling cycle.

Stabilisation of tetrabromo- and tetrachlorosemiquinone (bromanil and chloranil) anion radicals in crystals

Alkali salt crystals of the tetrahalogeno-semiquinone anion radical acetone solvates

and their solvent-free salts were studied by a combination of single-crystal X-ray diffraction, EPR spectroscopy and ab initio quantum chemical calculations. A pair of π -stacked radical anion rings was described, with centroid separation distances of about 3.2 Å and carbon-carbon contacts between the contiguous rings 0.3 Å shorter than the sum of van der Waals radii, enabling spin coupling of unpaired electrons. Therefore, these crystals are diamagnetic. Upon heating, the crystal structure of the acetone solvates, collapses and the sample turns paramagnetic - the electron spins of contiguous radicals decouple due to a loss of 3D ordering (Molčanov et al., 2011).

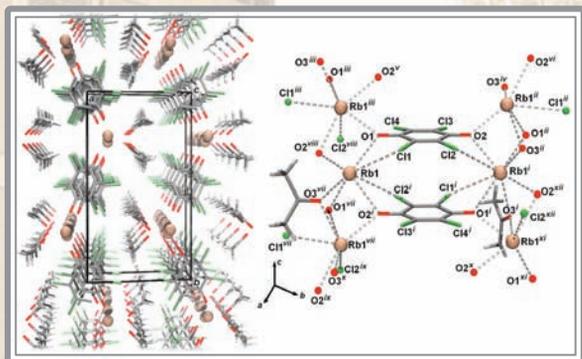


Fig 4. a) Crystal packing of a rubidium salt of tetrachlorosemiquinone radical anion, solvated with acetone. b) A cation-tethered diamagnetic (paired spins) dimer of semiquinone radical anions.

Validation of the catalytic mechanism of *Escherichia coli* purine nucleoside phosphorylase by structural and kinetic studies

The catalytic mechanism of *Escherichia coli* purine nucleoside phosphorylase (PNP) was examined using site-directed mutagenesis, kinetic studies and structure determinations. Five active site mutants were prepared. The crystal structures of the wild type enzyme in complex with phosphate/sulphate, and the Arg24Ala mutant in complex with phosphate/sulphate were determined. The crystal structures of the wild type enzyme complexes with phosphate and sulphate were determined as well as the crystal structure of Arg24Ala



Fig 5. The active site of the Arg24Ala mutant. In the wild-type protein active sites can be in both open and closed conformations, while in the mutated protein only the open conformation of the active site is observed.

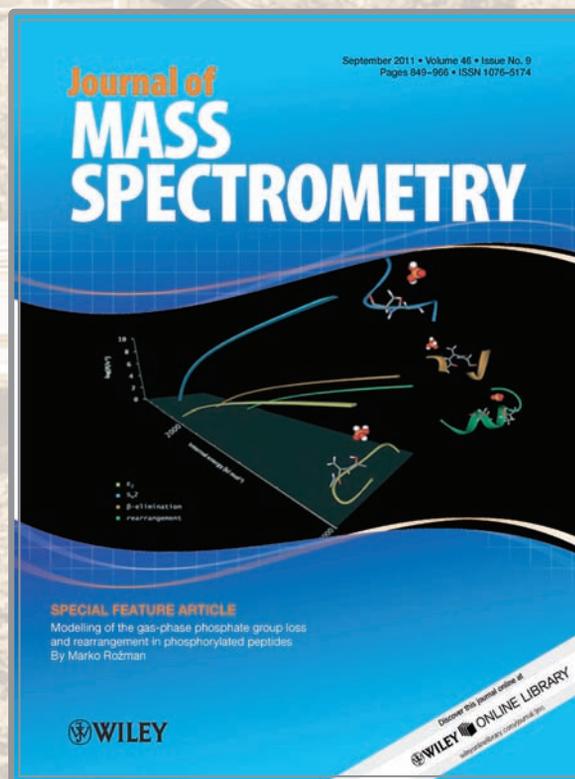


Fig 6. The front cover of the September issue of the Journal of Mass Spectrometry describing the energetic and kinetic aspects of the gas-phase unimolecular dissociation of phosphorylated peptides.

mutant complex with phosphate or sulphate (Mikleušević et al., 2011).

Modelling of gas-phase phosphate group loss and rearrangement in phosphorylated peptides

Phosphorylation is a key reversible protein posttranslational modification that regulates enzymatic activity, subcellular localization, complex formation and degradation of proteins. The molecular modeling work presented in this special feature article provides insight into the energetic and kinetic aspects of the gas-phase unimolecular dissociation of phosphorylated peptides. The elucidation of the proper phosphopeptide fragmentation behavior is of significant importance in the context of predicting tandem MS ion abundances (Rožman, 2011). An illustration summarizing these important results (Figure 6) appeared on the front cover of the September issue of the Journal of Mass Spectrometry.

NEW EQUIPMENT

The Division houses a mass spectrometry facility which has been upgraded with the acquisition of two new mass spectrometers (Bruker Daltonics, MS (ion trap) amaZon ETD and MS MALDI TOF Microflex LT/SH) for the analysis of proteins. The available technologies include mass spectrometers coupled with MALDI and ESI ion sources, autosampler and nano-2D-UHPLC system for high resolution separation of proteolytic peptides. Protein identification and full characterization of structure is achieved by an on-line, hyphenated liquid chromatography and mass spectrometry platform. Availability of the nano-spray ionization technique enables the analysis of proteins at the picomole level, which is of particular importance for low abundance samples. This biological mass spectrometry upgrade provides Croatian researchers access to a new range of experimental solutions critically important in

chemistry, environmental and life science research.

EDUCATION

Division members provided more than 30 undergraduate and graduate courses at Universities in Zagreb, Split, Rijeka, Osijek and Dubrovnik.

AWARDS

1. Manda Ćurić and Marina Juribašić: RBI Director's Prize for publishing in high ranking journals.
2. Darija Jurašin: Postdoctoral Fellowship from the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia (UKF grant): Characterization of biopolymeric scaffolds interaction with cells (01.06.2011 – 30.11.2011).

PROJECTS

Program supported by the Ministry of Science, Education and Sport

1. Molecular structure, dynamics and reactivity. Program leader: Boris Rakvin

Projects supported by the Ministry of Science, Education and Sport

1. Molecular structure and dynamics of systems with paramagnetic particles, Boris Rakvin
2. Surfactants, processes in solutions and at interfaces, Maja Dutour Sikirić
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, Manda Ćurić

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, Darko Babić
12. Amino-beta-lactams-synthrons for biologically interesting compounds, Ivan Habuš
9. Sythesis, structure, and antifungla activity of novel dithiocarbamato EDTA derivatives and their metal complexes, A. Višnjevac (Bilateral project with Montenegro)
10. A biomimetic approach towards the design of a novel peptide deformylase inhibitor, A. Višnjevac (HAZU project)
11. Single crystals of organic stable radicals as EPR probes at the surface of the single-molecule magnet Mn12-acetate, D. Žilić (HAZU project)

Research, developmental and international projects

1. Excited states of peptides in gas phase, I. Ljubić (Bilateral project with France, Program "COGITO")
2. Laser controlled switching of molecular photonic wires, N. Došlić (Bilateral project with Germany)
3. The study of condensed matter by EPR: Dynamics in glassy and crystalline matrices, M. Ilakovac Kveder (AvH research group linkage project)
4. Supramolecular chemistry in water, M. Ilakovac Kveder (COST CM1005)
5. Mass spectrometry-based proteomic analysis: Characterisation of horseradish esterases and snake venom proteins, and mapping of *Fusarium parasites*, I. Leščić Ašler (Bilateral project with Austria)
6. Synthesis, identificatrion and biological activity testing of novel beta lactam cholesterol absorption inhibitors, I. Habuš (Bilateral project with Austria)
7. Synthesis of amorphous calcium phosphate by ultrasonic spray pyrolysis, M. Dutour Sikirić (Bilateral project with Serbia)
8. Distributed simulation of biomolecular dynamics on a computing grid, N. Došlić (Bilateral project with Serbia)

SELECTED INVITED LECTURES

1. Ljubić I (2011) Theory as a guidance for the interpretation and planning of experiments. Commissariat de Recherche Atomique (CEA), Saclay, France, March 15, 2011.
2. Ljubić I (2011) Dynamics of reversible hydrogen storage in titanium doped sodium aluminium hydride. «Japanese-Croatian Workshop on Materials Science», Institute of Physics, Zagreb, October 6-7 2011.
3. Klasinc L (2011) Photochemical pollution indicators from ozone data. «43rd IUPAC World Chemistry Congress», Puerto Rico, Puerto Rico, July 30 – August 7, 2011.
4. Tomić S (2011) Molecular modelling on metalloenzymes. Heidelberg Institute for Theoretical Studies, Heidelberg, Germany, December 15, 2011.

SELECTED PUBLICATIONS

1. Cinčić D, Juribašić M, Babić D, Molčanov K, Šket P, Plavec J, Čurić M. New insight into solid-state molecular dynamics: Mechanochemical synthesis of azobenzene/triphenylphosphine palladacycles. *Chem Commun* **47** (2011) 11543.
2. Došlić N, Gomzi V, Mališ M, Matanović I, Eckert J. Fluxionality of hydrogen ligands in $\text{Fe}(\text{H})_2(\text{H}_2)(\text{PEtPh}_2)_3$. *Inorg Chem* **50** (2011) 10740.
3. Jurašin D, Pustak A, Habuš I, Šmit I, Filipović-Vinceković N. Polymorphism and mesomor-

- phism of oligomeric surfactants: Effect of the degree of oligomerization. *Langmuir* **27** (2011) 14118.
- Arh G, Klasinc L, Veber M, Pompe M. Calibration of mass selective detector in non-target analysis of volatile organic compounds in the air. *J Chromatogr A* **1218** (2011) 1538.
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 - Molčanov K, Sabljic I, Kojić-Prodić B. Face-to-face π -stacking in the multicomponent crystals of chloranilic acid, alkali hydrogenchloranilates, and water. *CrystEngComm* **13** (2011) 4211.
 - Juribašić M, Bellotto L, Traldi P, Tušek-Božić Lj. Electrospray ionization mass spectrometry of palladium(II) quinolinylaminophosphate complexes. *J Am Soc Mass Spectr* **22** (2011) 1815.
 - Miklušević G, Štefanić Z, Narczyk M, Wielgus-Kutrowska B, Bzowska A, Luić M. Validation of the catalytic mechanism of Escherichia coli purine nucleoside phosphorylase by structural and kinetic studies. *Biochimie* **93** (2011) 1610.
 - Churchard AJ, Banach E, Borgschulte A, Caputo R, Chen JC, Clary, David C, Fijalkowski KJ, Geerlings H, Genova RV, Grochala W, Jaroń T, Juanes-Marcos JC, Kroes GJ, Ljubić I, Naujoks N, Nørskov JK, Olsen RA, Pendolino F, Remhof A, Románszki L, Tekin A, Vegge T, Zäch M, Züttel A. A multifaceted approach to hydrogen storage. *Phys Chem Chem Phys* **13** (2011) 16955.
 - Rožman M. Modelling of the gas-phase phosphate group loss and rearrangement in phosphorylated peptides. *J Mass Spectrom* **46** (2011) 949.
 - Škorić I, Kikaš I, Kovács M, Fodor L, Marinić Ž, Molčanov K, Kojić-Prodić B, Horváth O. Synthesis, photochemistry and photophysics of butadiene derivatives: influence of the methyl group on the molecular structure and photoinduced behavior. *J Org Chem* **76** (2011) 8641.
 - Rožman M, Schneider A, Gaskell SJ. Proton transfer reactions for improved peptide characterisation. *J Mass Spectrom* **46** (2011) 529.
 - Juribašić M, Molčanov K, Kojić-Prodić B, Bellotto L, Kralj M, Zani F, Tušek-Božić Lj. Palladium(II) complexes of quinolinylaminophosphonates: Synthesis, structural characterization, antitumor and antimicrobial activity. *J Inorg Biochem* **105** (2011) 867.
 - Kveder M, Jokić M, Rakvin B. Fast motion in molecular solids at low temperatures: evidence from a pulsed EPR study of nitroxyl radical relaxation. *J Chem Phys* **134** (2011) 044531.
 - Ljubić I, Sabljic A. CASSCF/CASPT2 and TD-DFT study of valence and Rydberg electronic transitions in fluorene, carbazole, dibenzofuran, and dibenzothiophene. *J Phys Chem A* **115** (2011) 4840.

Division of Organic Chemistry and Biochemistry

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

ZOKB

DIVISIONAL ORGANIZATION

Head: Kata Majerski

The Division of Organic Chemistry and Biochemistry (DOCB) 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, Lidija Varga-Defterdarović
- ⇒ Laboratory for cellular biochemistry, Marija Abramić
- ⇒ Laboratory for physical organic chemistry, Davor Margetić
- ⇒ Laboratory for molecular spectroscopy, Goran Baranović
- ⇒ Laboratory for study of interactions of biomacromolecules, Ivo Piantanida
- ⇒ Group for quantum organic chemistry, David Smith



scientific articles were published, primarily in high-ranking chemical journals. Amongst the broad range of topics covered, important contributions were made in areas such as: synthetic and physical organic chemistry, stereoselective synthesis, supramolecular chemistry, including gels and host-guest interactions, the interactions of small molecules with DNA/RNA, the chemistry of peptides and peptidomimetics, molecular spectroscopy; experimental and computational protein biochemistry, the structure-function relationship and catalytic mechanism of metallopeptidases and quantum organic chemistry. In addition to fundamental research, one patent application was approved. Members of the Division provided significant contributions to higher education by providing numerous courses at the undergraduate and doctoral levels as well as by supervising 9 Master theses and 6 Ph.D theses. The Division's staff was also active in national and international societies and bodies and served as editors or members of several editorial boards.

OVERVIEW OF THE DIVISION

In 2011, members of the Division continued to maintain their established excellence in scientific research. The principal focus was directed towards basic research in the fields of organic and bioorganic chemistry. Over 59

Intense Optical Activity from Three-Dimensional Chiral Ordering of Plasmonic Nanoantennas

A record level of optical activity interpreted as surface plasmon CD (SP-CD) was obtained from a nano-composite containing a chiral assembly of nano-rods (NR) adsorbed onto helical gel fibers through specific non-covalent interactions. The use of such plasmonic nano-antennas as chirality probes upon attachment to proteins or DNA for in situ structure determination is anticipated and additional applications may include non-linear optics, negative refraction, and surface-enhanced Raman optical activity (Guerrero-Martinez et al., 2011).

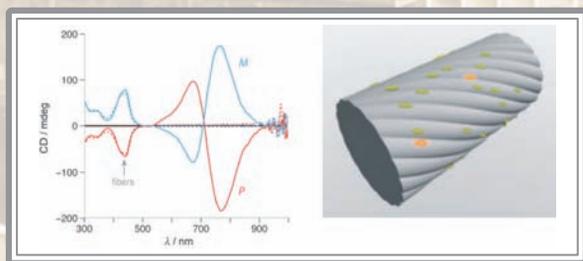


Fig. 1. Experimentally determined surface plasmon CD (SP-CD) of gold nano-rods adsorbed onto gel fibers of opposite helicity.

Prediction of novel organic superbases

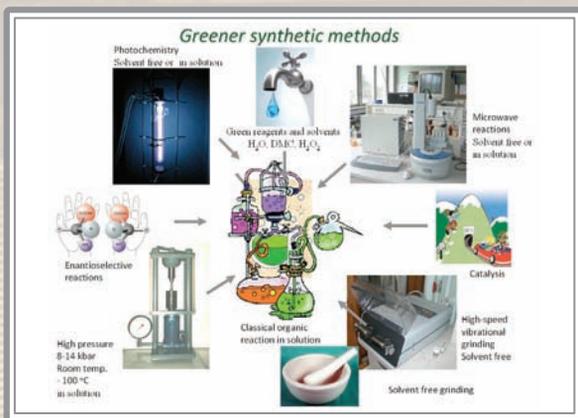


Fig. 2. Green synthetic methods

Computational methods revealed that several conjugated polycyclic organic frame-

works formed skeletons for extremely basic compounds, some of which exceed gas-phase proton affinities of $PA = 300 \text{ kcal mol}^{-1}$ and 40 pK_a units in acetonitrile. The high values are due to the formation of a hydrogen bond upon protonation and an efficient cationic resonance in the conjugate acids (Peran et al., 2011).

Modeling the vibrational spectra of molecules in condensed phase

An efficient computational procedure was developed to model the vibrational spectra of a physiologically relevant histamine mono-cation in aqueous solution. The results revealed excellent agreement with experimental findings and showed that the ring amino group absorbs at higher frequencies than the remaining three amino N-H protons of the protonated aminoethyl group. In this way the results of the simulation complemented the experimental spectrum that cannot distinguish between the two sets of protons. The proposed methodology represents a powerful tool for the computational support of vibrational spectroscopy (Stare et al., 2011).

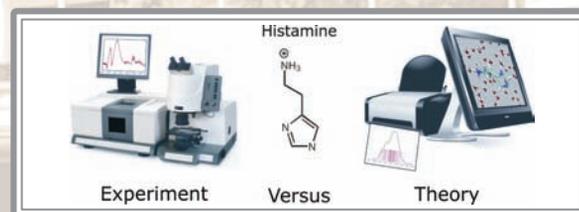


Fig. 3. Excellent agreement between theory and experiment resolves mysteries in the vibrational spectra of histamine mono-cation

Synthesis, photochemistry and quantum-chemical study of the $(8\pi, 6\pi)$ -electrocyclisation of [3,4]-benzo-8-methyl-(E,Z,Z,E)-1,3,5,7-octatetraene

The first example of thermal $(8\pi, 6\pi)$ -electrocyclisation of 1,3,5,7-octatetraene with one double bond embedded in an aromatic moiety is described. Through this process, [3,4]-benzo-8-substituted octatetraene derivatives were transformed into new endo-

7- and exo-7-substituted-2,3-benzobicyclo[4.2.0]octa-2,4-dienes. The mechanism of this reaction was also studied by DFT quantum-chemical calculations, which indicated that formation of the single endo- isomer in the case of phenyl and 2-furyl substituents is determined by higher activation barriers for exo-6 π -electrocyclisation than for 8 π -cycloversion (Škorić et al., 2011).

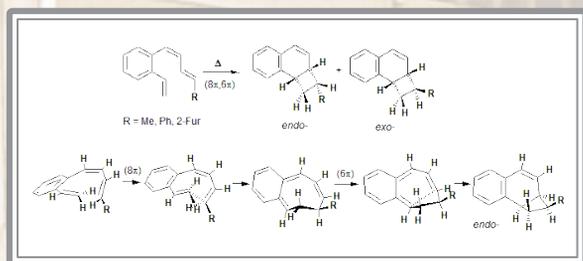


Fig. 4. Thermal (8 π ,6 σ)-electrocyclisations of 1,3,5,7-octatetraenes

Advances in the development of single molecule-multipurpose sensors for simultaneous differentiation of various DNA/RNA forms

Further progress in studies of DNA/RNA active small organic molecules resulted in 9 new scientific publications, among which the most intriguing result was efficient differentiation between dGdC, dAdT and rArU sequences by a single molecule, acting as a multi-purpose marker (Radić Stojković et al., 2011).

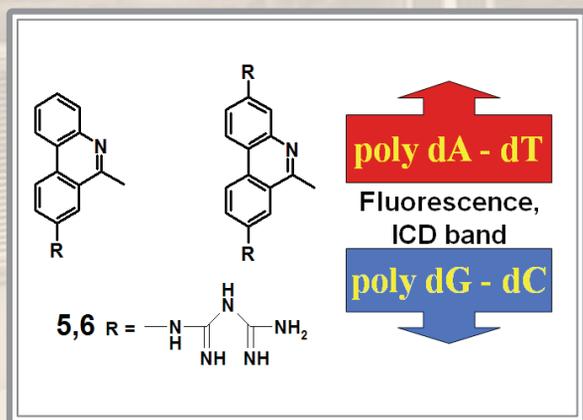


Fig. 5. The phenanthridine biguanides efficiently differentiate between dGdC, dAdT and rArU sequences by two independent, sensitive spectroscopic methods

Ab initio quantum dynamical study of the multi-state nonadiabatic photodissociation of pyrrole yields bond dissociation probabilities

Ab initio based quantum dynamical investigation of the photodynamics of pyrrole by surface hopping techniques was extended to cover simultaneously the lowest five singlet states. The results reveal a sub-picosecond internal conversion from the S₄ ($\pi - \pi^*$) state, corresponding to the strongly dipole-allowed transition, to the S₁ and S₂ ($\pi - \sigma^*$) states and to the ground state of pyrrole. The first results for the dissociation probabilities of the three lowest electronic states were also presented (Faraji et al., 2011).

Stereochemistry of 2,6-Diaminoadamantane Salts: Transannular Interactions

New adamantane-2,6-diammonium salts were prepared and their solid state stereochemistry was studied. The crystal structure of the rac-N,N,N',N'-tetramethyl-2,6-diaminoadamantane dihydrochloride salt (3) contained a 2.5 hydrate with two molecules of opposite handedness in the asymmetric unit ($Z' = 2$) related by pseudo-inversion. In this crystal structure there is an unusual hydrogen bonding arrangement. For each molecule in the asymmetric unit, one of the two dimethylammonium +N-H units is hydrogen-bonded to a chloride anion, while the second +N-H is hydrogen-bonded to the water oxygen (Glaser et al., 2011).

Paving the way for new drugs against Parkinson disease

Quantum-chemical simulations elucidated the most feasible mechanism of the irreversible inhibition of Monoamine oxidase B by the acetylenic inhibitors rasagiline and selegiline, which are both used to relieve symptoms of Parkinson disease. This is a prerequisite for the design and synthesis of novel anti-parkinsonians. Artwork from this

publication was selected for the cover of the European Journal of Organic Chemistry (Borštnar et al., 2011).

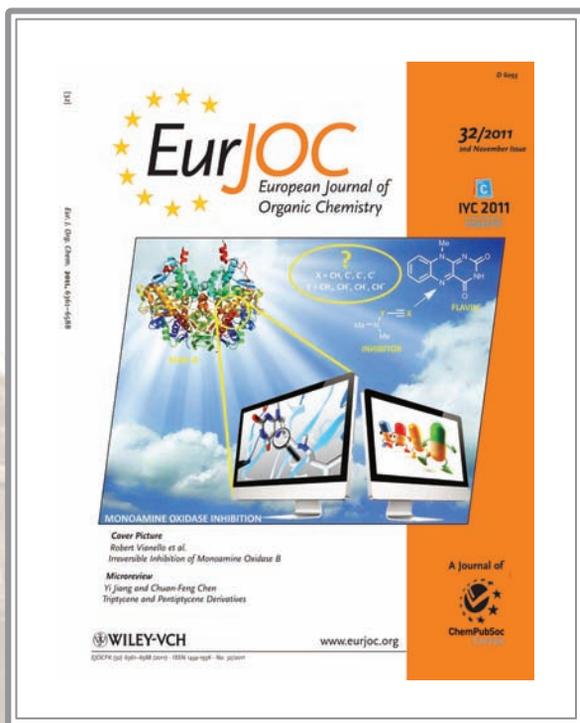


Fig. 6. Cover page of the European Journal of Organic Chemistry 32/2011 depicting the mechanism of the inhibition of MAO enzymes by acetylenic drugs

Ligand binding to human dipeptidyl peptidase III

To understand the mode of ligand binding into the active site of human dipeptidyl peptidase III, a zinc peptidase involved in protein biosynthesis and defense against oxidative stress, a combined experimental and computational approach was applied. The mutation of the conserved His568 resulted in a 1300-fold decrease of k_{cat} , and in lowered affinity for the competitive inhibitor, while the MD simulations of the wild-type and H568N protein variant revealed key enzyme-ligand interactions and ligand-induced reorganization of the binding site (Tomić et al., 2011).

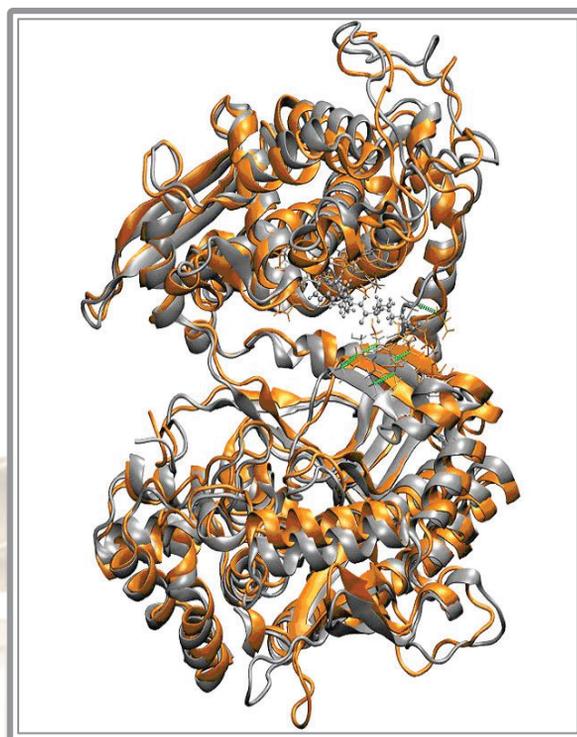


Fig. 7. Structure of human DPP III after 10 ns of productive MD simulations of the free enzyme (orange) and of DPP III complex with substrate (silver). Five green dotted lines represent shifts in position of Asp372, Gly389, Asn391, Asn406 and Ser408.

Domino Diels–Alder reactions of N-methoxyethyl-7-oxanorbornadiene-2,3-dicarboximide: an elusive, highly reactive dienophile

Flash vacuum pyrolysis (FVP) has been used to generate a novel 7-oxa-norbornadiene-2,3-dicarboxylic imide that, in situ, gave an unprecedented cycloaddition reaction cascade with the imidofuran, a side-product of FVP. Stereoselectivity of cycloadditions was studied with the aid of density

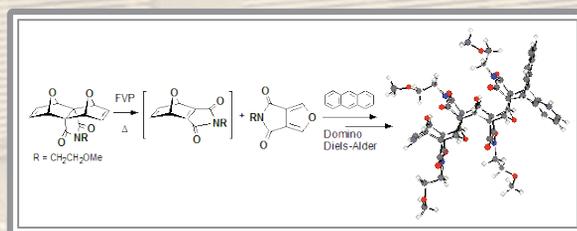


Fig. 8. Domino Diels–Alder reactions of N-methoxyethyl-7-oxanorbornadiene-2,3-dicarboximide

functional calculations, which fully support the observed exo/endo-selectivity (Margetić et al., 2011).

Phosphate selective alkylenebisurea receptors: Structure-binding relationship

New host molecules for the anions, adamantane and alkyl urea derivatives substituted by naphthalene chromophores, were synthesized. Their binding with F^- , Cl^- , Br^- , OAc^- , HSO_4^- , NO_3^- and $H_2PO_4^-$ was investigated by UV-Vis, fluorescence and NMR spectroscopy and by microcalorimetry. The strongest binding is observed with $H_2PO_4^-$ and F^- . The titrations with anions suggested that complexes in solution are probably present in a dynamic equilibrium of many conformations (Blažek et al., 2011).

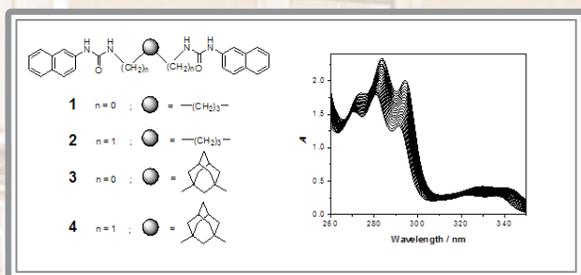


Fig. 9. UV-vis titration of **3** with $H_2PO_4^-$ in CH_3CN . The bottom curve corresponds to the solution of **3**, whereas the curves from bottom to up correspond to the solutions with increasing concentration of $Bu_4NH_2PO_4$.

Analysis of opiorphin in human saliva

Opiorphin, QRFSR-peptide, is a mature product of the Prol1 protein that showed beneficial effects in pain management, antidepressant-like actions as well as involvement in colonic motility and erectile physiology. Using opiorphin as a potential biomarker of different pathological states requires the development of robust and sensitive methods. We report a highly sensitive and specific liquid chromatography with tandem mass spectrometric detection (LC-MS/MS) ana-

lytical method for the analysis of opiorphin in human saliva (Brkljačić et al., 2011).

Synthesis of new chiral building blocks with double functionality

As part of our ongoing research of brush-type chiral stationary phases we developed the synthesis of a series of chiral selectors containing a terminal double bond, required for binding to silica surface. Chiral 1-aryl-allylamines have been recognised as key intermediates in this synthetic pathway and they were prepared with moderate to excellent enantioselectivities. The double functionality classifies enantio-enriched allyl amines as extremely interesting chiral building blocks with a wide range of further synthetic applications (Knežević et al., 2011).

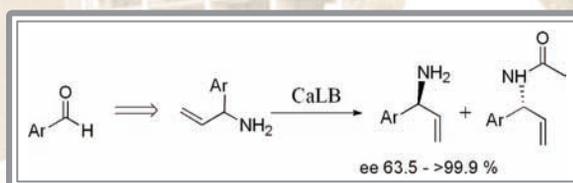


Fig. 10. Enzymatic approach to (S)-1-aryl-allylamines

Predicting antitumor activity of compounds using regression models

Predicting antitumor activity of compounds using regression models trained on a small number of compounds with measured biological activity is an ill-posed inverse problem. To counteract, up to some extent, overfitting

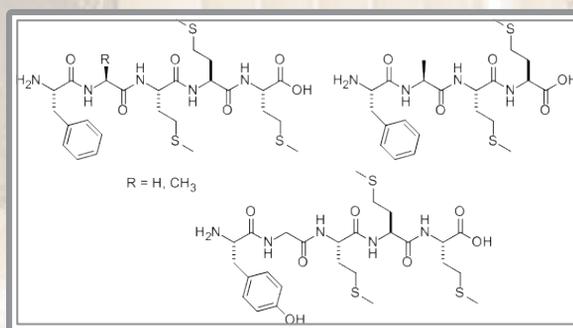


Fig. 11. Methionine-rich peptides obtained by the consensus of regression models.

problems caused by a small training data set, we used the consensus of six regression models for prediction of biological activity in a virtual library of compounds. The highly ranked candidate compounds were synthesized, characterized and tested for an antiproliferative activity (Radman et al., 2011).

PATENT

US patent: 8,022.097. Basarić N, Alešković M, Majerski K. Adamantane-dipyrromethane derivatives, method of preparation and applications in anion sensing.

SPIN OFF COMPANY

BioZyne Ltd. was re-launched in 2010/2011 with a new strategy for the company's research and development in life sciences. The company's vision is to take steps towards the creation of an anticancer research centre for Croatia. BioZyne Ltd. is to provide optimized active lead compounds as potential drug molecules for the treatment of cancer. Those active leads are expected to result from compounds protected by RBI's European patent - EP0877022B1 and other novel and promising compounds that will result from the know-how and technologies of the RBI research team.

NEW EQUIPMENT



Fig. 12. Planetary mill Retsch PM200

In the Laboratory for physical organic chemistry a new Planetary mill Retsch was installed.

EDUCATION

Members of the Division provided significant contributions to higher education by providing numerous courses at the undergraduate and doctoral levels at the Universities: Zagreb, Rijeka, Osijek, Split and Dubrovnik. Members of DOCB are involved in several PhD programs, in particular, Chemistry – PhD program at the Faculty of Science, University of Zagreb; Medicinal Chemistry – PhD Program at the University of Rijeka, and Chemistry of Mediterranean Environment – PhD Program at the University of Split.

AWARDS

1. Award to Marija Alešković: 2011 RBI director general's award for recognition of international patent US 8,022.097.
2. Award to Karmen Čondić-Jurkić: WATOC Poster Prize awarded at the 9th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2011), Santiago de Compostela, Spain, July 16–22, 2011.
3. Award to Nena Radić (Peran): Best Poster Prize awarded at the 13th European Symposium on Organic Reactivity (ESOR XIII), Tartu, Estonia, September 11–16, 2011.
4. Award to Nena Peran: 2011 RBI director general's award for a scientific publication with high impact factor.
5. Award to Andreja Radman: Krka Prize Winner for Diploma Thesis (International award given by pharmaceutical company Krka, Novo Mesto, Slovenia).
6. Award to Vjekoslav Štrukil: CrystEngComm award for poster "Mechanochemical Synthesis of Zinc and Cadmium Metal-Organic Frameworks - The Story of Dimensionality and Solid-State Reactivity" presented at XX

International Conference on the Chemistry of the Organic Solid State, June 26-30, 2011, Bangalore, India.

- Award to Pavle Trošelj: National science foundation program for education of doctoral students „Doctoral students scholarships“ - group prof. Koji Nakanishi, prof. Nina Berova, Columbia University, NY, USA, September 1, 2011 – January 31, 2012.

- Macrocyclic ligands, structures in solutions and molecular spectroscopies, Goran Baranović
- Design, synthesis and study of interactions of small molecules with DNA, RNA and proteins, Ivo Piantanida
- Brönsted and Lewis acids and bases in chemistry and biochemistry, Zvonimir Maksić/Robert Vianello.
- Computational studies of protein structure and function, David Smith.

PROJECTS

Programs supported by the Ministry of Science, Education and Sport

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

Projects supported by the Ministry of Science, Education and Sport

- Chiral building blocks for biological active molecules. Synthesis and reactivity, Zdenko Hameršak
- Chiral organic materials - synthetic, structural and functional research, Vladimir Vinković
- Cage Compounds: Building Blocks for Molecular Architecture, Kata Majerski
- Self-assembly in gels and synthesis of functional hybrid materials, Mladen Žinić
- Synthesis of novel biologically active nucleobase and nucleotide derivatives, Biserka Žinić
- Chemical transformations of natural compounds; Lidija Varga-Defterdarović
- Molecular enzymology and protein interactions of hydrolases, Marija Abramić
- 'Host-guest' interactions in polycyclic systems, Davor Margetić
- Organic and bioorganic processes in ground and electronically excited states, Mirjana Maksić

Research, developmental and international projects

- Biocatalytic application of halohydrin dehalogenases for production of chiral building blocks. Maja Majerić Elenkov, UKF 3A Grant Agreement 51/09.
- Photochemistry of polycyclic molecules: From mechanistic studies to new drugs and medicinal applications. Nikola Basarić, HRZZ 02.05/25.
- Mechanochemistry for the clean and efficient metal-catalysed synthesis of pharmaceutical targets and the study of their molecular recognition. Mirjana Maksić, Unity Through Knowledge Fund, 1B Grant Agreement 63/10).
- Artificial Receptors for Bacillus anthracis Specific Anthrose Detection. Andreja Jakas and Predrag Cudic, NATO Science for Peace and Security Programme; CBP.EAP.SFP.983154.
- Computational studies of proton dynamics in hydrogen bonded systems and enzymes. Robert Vianello, individual Marie Curie Intra-European Fellowship for career development (European Commission, FP7-PEOPLE-2009-IEF call, 2010-2012).
- Fluorescent Anion Sensors: Synthesis and Spectroscopic Characterization. Nikola Basarić, Bilateral project Croatia - P.R. China, 2009 – 2011.
- Photoactive nano-structured gel systems with controlled optical properties. Mladen Žinić, Bilateral project COGITO, Croatia- France, 2011 – 2012.
- Semirational design of halohydrin dehaloge-

- nase HheA for its application in the synthesis of chiral building blocks. Maja Majerić Elenkov, Bilateral project Croatia - P.R. China, 2011-2013.
- Structure – function relationship in metallo-peptidase family M49. Marija Abramić, Bilateral project Croatia – Austrija, 2010-2011.
 - Gas-phase studies on novel guanidines as superbases and as bifunctional receptors. Bilateral project DAAD, Croatia-Germany, 2011-2012,

SELECTED INVITED LECTURES

- Vianello R. From the laboratory of Marie Skłodowska Curie for a brighter future of mankind. "Science Festival 2011", Rijeka, Croatia, April 11–15, 2011.
- Maksić, M. Formamide as the model compound for photodissociation of the peptide bond, Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists, Yáñez, Manuel ; Mó, Otilia (ed.). Santiago de Compostela, July 16–22, 2011.
- Smith DM. The activation of coenzyme B₁₂. "The Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2011)", Santiago de Compostela, Spain, July 16–22, 2011.
- Basarić, N. Formation of sterically congested quinone methides in photodehydration of phenols. College of Chemistry and Chemical Engineering Lanzhou University, Lanzhou, P. R. China, August 4, 2011.
- Basarić N, Bobinac D, Cindro N, Mlinarić-Majerski K, Uzelac L, Kralj M, Wan P. Characterization of sterically congested biphenyl quinone methides and zwitterions by laser flash photolysis, and investigation of their antiproliferative activity. „International Conference on Photochemistry ICP 2011“, Beijing, P.R. China August 7-12, 2011.
- Vianello R. Hydrogen bond dynamics and computational vibrational spectroscopy in aqueous solution: the case study of histamine monocation. "XVIth International Workshop on Quantum Systems in Chemistry and

- Physics (QSCP–XVI)", Kanazawa, Japan, September 10–17, 2011
- Maksić M. Guanidines from theory and synthesis to applications. Institute for Organic chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic, October 11, 2011.
- Margetić D, Štrukil V, Eckert-Maksić M, Igrc M.D, Friščić T, Fábíán L, Reid D.G, Duer M.J, Jackson G.J. Mechanochemistry - environmentally friendly method for modification and synthesis of pharmaceuticals. Faculty of pharmaceutical sciences, Musashino University, Tokyo, Japan, December 20, 2011.

SELECTED ORGANIZED CONFERENCES

- Ruđer Josip Bošković Physicist and Astronomer, Symposium, Zagreb, May 25, 2011 (organizer Mirjana Maksić)

SELECTED PUBLICATIONS

- Guerrero-Martinez A, Auguie B, Alonso-Gomez JL, Džolić Z, Gomez-Grana S, Žinic M, Cid M M, Liz-Marzan LM. Intense Optical Activity from Three-Dimensional Chiral Ordering of Plasmonic Nanoantennas. *Angew Chem Int Ed* **50** (2011) 5499.
- Peran N, Maksić ZB. Polycyclic croissant-like organic compounds are powerful superbases in the gas phase and acetonitrile – a DFT study. *Chem Commun* **47** (2011) 1327.
- Dörr FA, Kovačević B, Maksić ZB, Ernani P, Volmer DA. Intriguing Differences in the Gas-Phase Dissociation Behavior of Protonated and Deprotonated Gonyautoxin Epimers. *J Am Soc Mass Spectrometry* **22** (2011) 2011.
- Stare J, Mavri J, Grdadolnik J, Zidar J, Maksić ZB, Vianello R. Hydrogen bond dynamics of histamine monocation in aqueous solution: Car-Parrinello molecular dynamics and vibrational spectroscopy study. *J Phys Chem B* **115** (2011) 5999.
- Wernersson E, Heyda J, Vazdar M, Lund

- M, Mason P, Jungwirth P. Orientational Dependence of the Affinity of Guanidinium Ions to the Water Surface. *J Phys Chem B* **115** (2011) 12521.
- Škorić I, Pavošević F, Marinić Ž, Šindler M, Eckert-Maksić M, Vazdar M, Margetić D. Synthesis, photochemistry and quantum-chemical study of the $(8\pi,6\pi)$ -electrocyclisation of [3,4]-benzo-8-methyl-(*E,Z,Z,E*)-1,3,5,7-octatetraene. *Org Biomol Chem* **9** (2011) 6771.
 - Gröger K, Baretić D, Piantanida I, Marjanović M, Kralj M, Grabar M, Tomić S, Schmuck C. Guanidiniocarbonyl-pyrrole-aryl conjugates as nucleic acid sensors: switch of binding mode and spectroscopic responses by introducing additional binding sites into the linker. *Org Biomol Chem* **9** (2011) 198.
 - Radić Stojković M, Miljanić S, Mišković K, Glavaš-Obrovac Lj, Piantanida I. The phenanthridine biguanides efficiently differentiate between dGdC, dAdT and rArU sequences by two independent, sensitive spectroscopic methods. *Mol Biosystems* **7** (2011) 1753.
 - Supek F, Šumanovac Ramljak T, Marjanović M, Buljubašić M, Kragol G, Ilić N, Šmuc T, Zahradka D, Mlinarić-Majerski K, Kralj M. Could LogP be a principal determinant of biological activity in 18-crown-6 ethers? Synthesis of biologically active adamantane-substituted diaza-crowns. *Eur J Med Chem* **46** (2011); 3444.
 - Faraji S, Vazdar M, Reddy S.V, Eckert-Maksić M, Lischka H, Koeppl H. Ab initio quantum dynamical study of the multi-state nonadiabatic photodissociation of pyrrole. *J Chem Phys* **135** (2011) 154310.
 - Glaser R, Steinberg A, Šekutor M, Rominger F, Trapp O, Mlinarić-Majerski K. Stereochemistry of 2, 6-Diaminoadamantane Salts: Transannular Interactions. *Eur J Org Chem* **32** (2011) 3500.
 - Borštnar R, Repič M, Kržan M, Mavri J, Vianello R. Irreversible inhibition of monoamine oxidase B by the antiparkinsonian medicines rasagiline and selegiline: a computational study. *Eur J Org Chem* **32** (2011) 6419.
 - Tomić A, Abramić M, Špoljarić J, Agić D, Smith D.M, and Tomić S. Human dipeptidyl peptidase III: insights into ligand binding from a combined experimental and computational approach. *J Molec Recognit* **24** (2011) 804.
 - Margetić D, Butler DN, Warrener RN, Murata Y. Domino Diels-Alder reactions of 7-oxanorbornadiene-2,3-dicarboximide: an elusive, highly reactive dienophile, Y. *Tetrahedron* **67** (2011) 1580.
 - Blažek V, Nikola B, Mlinarić-Majerski K, Nikola B. Phosphate selective alkylenebisurea receptors: Structure-binding relationship. *Tetrahedron* **67** (2011) 3846.
 - Zimmermann B, Baranović G.. Thermal analysis of paracetamol polymorphs by FT-IR spectroscopies. *J Pharmaceut Biomed Anal* **54** (2011) 295.
 - Naumov P, Topcu Y, Eckert-Maksić M, Glasovac Z, Pavošević F, Kochunnonny M, Hara HJ. Photoinduced rearrangement of aromatic N-chloroamides to chloroaromatic amides in the solid state. Inverted $\pi_N-\Sigma_N$ occupational stability of amidyl radicals. *Phys Chem A* **115** (2011) 7834.
 - Brkljačić L, Sabalić M, Salarić I, Jerić I, Alajbeg I, Nemet I. Development and validation of a liquid chromatography – tandem mass spectrometry method for the quantification of opiorphin in human saliva. *J Chromatogr B* **879** (2011) 3920.
 - Knežević A, Landek G, Dokli I, Vinković V. Efficient enzymatic approach to (S)-1-aryl-allyl amines. *Tetrahedron: Asymmetry* **22** (2011) 936.
 - Radman A, Gredičak M, Kopriva I, Jerić I. Predicting antitumor activity of peptides by consensus of regression models trained on a small data sample. *Int J Mol Sci* **12** (2011) 8415.

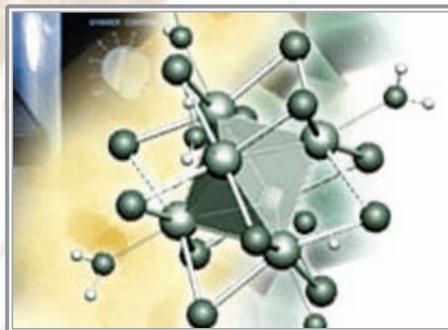


DIVISIONAL ORGANISATION

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
- ⇒ Laboratory for solid state and complex compounds chemistry, Pavica Planinić
- ⇒ Laboratory for ichtiopathology – biological materials, Rozelindra Čož-Rakovac



unit in Croatia covering all aspects of the physico-chemical effects of ionizing radiation and their applications. Low-dose and high-dose chemical dosimetry systems have been developed here and received international recognition. In addition, we undertake multidisciplinary research in which terrestrial or aquatic organisms are used as biomodels / biosensors for genotoxic impact of nanomaterials at the subcellular, cellular, tissue or organ level and this work is directed toward environmental, technological or medical applications. Our main research activities are financially sponsored by the Ministry of Science, Education and Sports.

OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is a centre of excellence in materials science. Our primary interests are in metal oxides, glass-ceramics, zeolites, slightly soluble ionic salts, cluster compounds, organic polymers, intermetallic compounds and metal hydrides. In vitro biomineralization processes are also the subject of research continuing a long tradition in the study of the mechanisms and kinetics of different precipitation systems. The Division's radiation chemistry and dosimetry laboratory is the only such

TOP ACHIEVEMENTS

New synthesis of hollow monodisperse hematite (α -Fe₂O₃) nanoparticles

This research demonstrates a unique experimental approach in the tailoring of α -Fe₂O₃ particles of desired size and morphology. Tailoring of specific hematite mor-

ologies is possible through the addition of inorganic ions or surface active agents into the precipitation systems (Gotić et al. 2011; Žic et al. 2011).

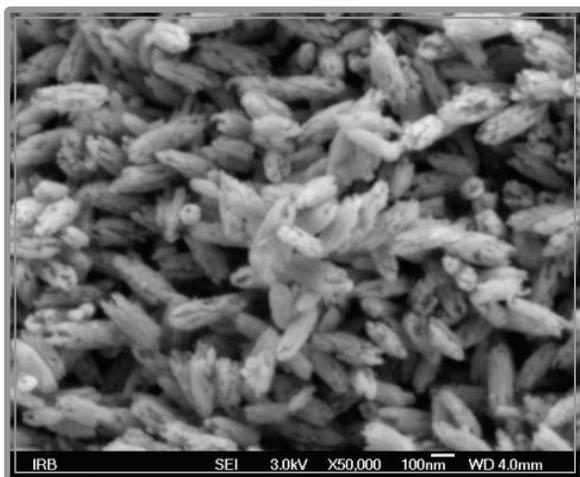


Fig. 1. Spindle-shape and hollow α - Fe_2O_3 particles.

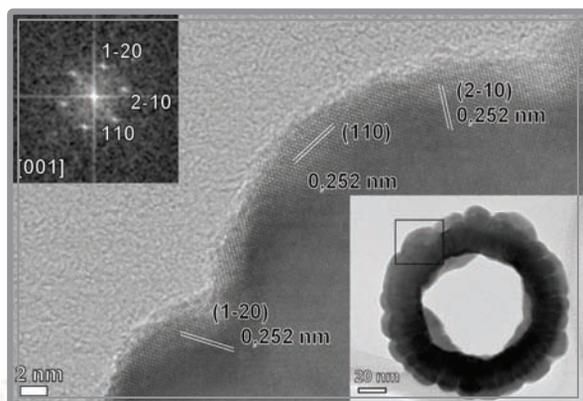


Fig. 2. α - Fe_2O_3 nanoring.

Further development of the theory of autocatalytic crystallization (nucleation)

Using kinetic data (rate of crystallization, rate of crystal growth) and crystal size distributions of zeolite A at the end of crystallization, the kinetics of nucleation and distribution of nuclei within the gel matrix were determined. The appearance of a large number of nuclei, at the moment when the gel is almost completely dis-

solved, was observed for the first time (Palčić et al., 2011).

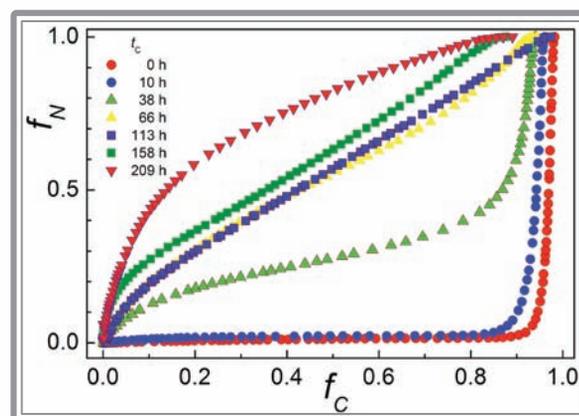


Fig 3. Changes in the distribution of the nuclei within gel matrix with ageing time of the starting hydrogel.

Theoretical study of magnetism in RM_{12}B_6 compounds (R = Y, La, or Ce; M = Fe, Co)

A DFT electronic structure study for RM_{12}B_6 intermetallics (R=Y, La or Ce; M=Fe, Co) was performed. Our results, including metamagnetic transition in $\text{LaFe}_{12}\text{B}_6$, are in fair agreement with previously obtained experimental and theoretical results (Miletić and Blažina, 2011).

Magnetic interactions in hexanuclear niobium and tantalum clusters

Magnetic interactions in the solid-state cluster compounds of niobium and tantalum have been determined experimentally and corroborated by DFT calculations. The interactions observed in compounds with one-dimensional structural motifs have been explained with the well-known Bonner-Fisher model (Fontaine et al., 2011), while those revealed in clusters showing three-dimensional diamond-like lattices (Fig. 3.) have been explained in the framework of the HTSE calculation (Perić et al., 2011).

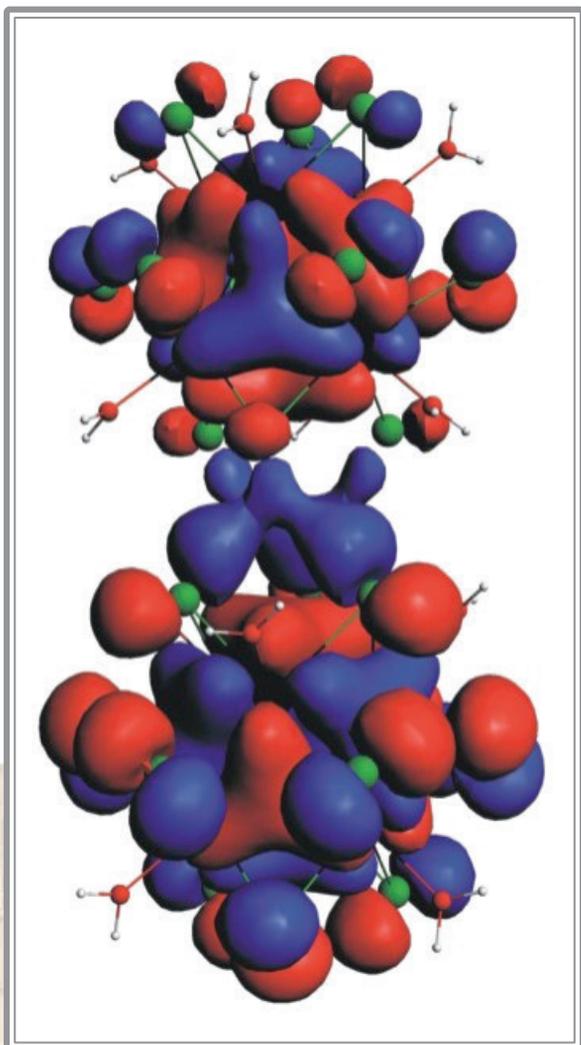


Fig. 4. SOMO orbital for the $[(Ta_6Br_{12}(H_2O)_8)_2]^{6+}$ dimer, equivalent to the pair of the nearest neighbouring clusters in $[NET_4] [Ta_6Br_{12}(H_2O)_8]Br_4 \cdot 4H_2O$. Significant overlap in the middle of the dimer is an evidence of the importance of the bridging halogen atoms in the magnetic exchange pathway.

Precipitation in hydrogels

Different carrageenan gelling environments were used as appropriate models for investigation of $CaCO_3$ precipitation, initiated at high initial supersaturation. The results indicated that the mineralogical composition, morphology and size distribution of the precipitate depended on the gelling status that was tuned by the carrageenan concentration and the addition of different cross-linking cations (Kosanović et al., 2011)

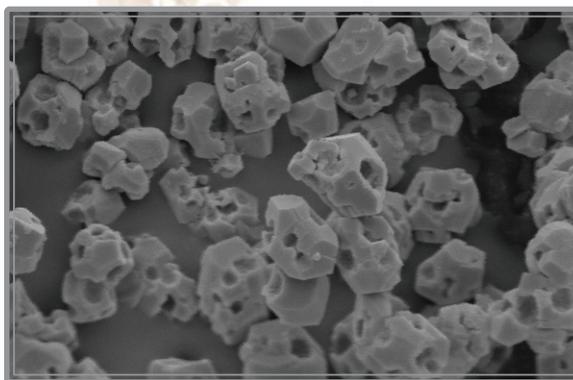


Fig. 5. SEM images of calcium carbonate precipitated in calcium carrageenan hydrogels.

Poly(ethylene oxide) irradiated in the solid state, melt and aqueous solution – a DSC and WAXD study

This study demonstrated that the aggregate state of PEO during irradiation is the most important factor in determining radiation outcome. Due to effective crosslinking, the irradiation of aqueous PEO solutions is the most suitable way to obtain PEO samples of a lower degree of crystallinity and phase transformation temperatures while preserving its mechanical properties (Jurkin et al., 2011).

Lipidomics

Lipid peroxidation and lipid isomerisation have been studied under biomimetic conditions. These two processes are compared for the first time, demonstrating that hydroperoxides and *trans* lipids are formed to comparable extents as a result of oxidative free radical conditions (Mihaljević et al., 2011).

Classification modelling of physiological stages in captive Balkan whip snakes using blood biochemistry parameters

Captive Balkan whip snakes (*Hierophis gemonensis*) were studied to determine blood biochemical parameters as potentially useful indicators of physiological status dur-

ing different periods of the biological cycle, including pre- and post-hibernation, hibernation, sexual activity, and normal activity using several machine-learning methods. This approach clarifies the role and importance of physiological processes which show diversity of functional characteristics of various biochemical parameters in ecological relation to snakes held under laboratory conditions which mimic natural environmental changes (Čož-Rakovac et al., 2011).

NEW EQUIPMENT

A high pressure liquid chromatographic system with a diode array detector (Agilent HPLC Infinity 1260) was purchased by a HrZZ funded project. The instrument will be used for the analysis and purification of metallated peptides, pseudo-peptides and peptide nucleic acids prepared by microwave assisted solid phase synthesis.



Fig. 6. High pressure liquid chromatograph

EDUCATION

In 2011, scientists and researchers from the Division contributed to the educational programs at the Universities in Zagreb, Osijek, Dubrovnik and Rijeka, conducting 18 undergraduate and postgraduate courses.

AWARDS

Award to Berislav Perić and Pavica Planinić: Annual Director's Award, Ruđer Bošković Institute (2011), was given for publishing one or more scientific papers in the journals with high impact factor in chemistry.

Award to Andrea Knežević, Trpimir Ivšić and Zoran Kokan: „Chiral molecule hygiene“, Best poster award in the category „Molecular Architecture“, Scientific Encounters of the Third Kind (Z3V), Ruđer Bošković Institute, 2011.

PROJECTS

Programs supported by the Ministry of Science, Education and Sports

1. New functional materials, Svetozar Musić

Projects supported by the Ministry of Science, Education and Sport

1. Synthesis and microstructure of metal oxides and oxide glasses, Mira Ristić
2. Study of influence of aluminosilicate precursors on their transformation, Boris Subotić
3. Precipitation mechanism of inorganic biocompatible and related materials, Damir Kralj
4. Metal hydrides in clean energy systems, Želimir Blažina
5. Polynuclear metal systems – synthesis and properties, Pavica Planinić
6. Structure-property relationships of modified polymer materials, Ivan Šmit
7. Physico-chemical effects of ionizing radiation in materials, Saveta Miljanić

8. Subcellular biochemical and phylogenetic diversity of aquatic organisms, Rozelindra Čoz-Rakovac

Research, developmental and international projects

1. Corals and global warming: The Mediterranean versus the Red Sea (CoralWarm) FP7 IDEAS – ERC Advanced Grant, Grant Agreement N. 249930, subcontract Damir Kralj (Task 5.4)
2. Nanoparticle cell interaction: Molecular signaling events induced by synthesized new nanomaterials. Marijan Gotić (Croatian-German bilateral project)
3. Synthesis and characterization of multi-metallic bioconjugates. Srećko Kirin (Croatian-German bilateral cooperation program)
4. Metallated bioconjugates for applications in biological and material sciences. Srećko Kirin (Homing program, Croatian science foundation HrZZ, 2010-2011)
5. Organometallic and inorganic bioconjugates as potential enantioselective catalysis. Srećko Kirin (Homeward program, Unity through knowledge fund UKF, 2009-2011)
6. Free Radicals in Chemical Biology (CHEM-BIORADICAL) COST CM 0603, Branka Mihaljević
7. Solid state detectors in mixed radiation fields dosimetry, Croatian-Hungarian Intergovernmental S&T Cooperation, Saveta Miljanić
8. Enhancing Quality Control Methods and Procedures for Radiation Technology, IAEA Regional Technical Co-operation Project RER 8/017, Saveta Miljanić
9. Radiation protection dosimetry in medicine: The risk of early and late health effects from the use of radiation therapy. EURADOS Working Group 9, Saveta Miljanić
10. European Medical ALARA Network (EMAN), EURADOS Working Group 12, Željka Knežević
11. Design of polymer blends and composites. Irina Pucić (Croatian-Slovenian bilateral project)
12. Interactions in radiation modification of

poly(ethylene oxide) and its nanocomposites. Irina Pucić (Croatian-Hungarian bilateral project)

13. Radiation synthesis and characterization of nanomaterials for health care, environmental protection and clean energy applications, IAEA Regional Technical Co-operation Project, Tanja Jurkin and Irina Pucić
14. The effects of high-energy radiation on polymeric systems, Croatian-Hungarian Intergovernmental S&T Cooperation, Irina Pucić
15. Using Nuclear Techniques for the Characterisation and Preservation of Cultural Heritage Artefacts in the Europe Region, IAEA RER/8/015, Branka Katusin-Ražem
16. Scientific cooperation between Ruđer Bošković Institute and Chiyoda Technology, Japan. Saveta Miljanić, Marija Ranogajec-Komor, Željka Knežević.

SELECTED INVITED LECTURES

1. Bronić J (2011) Particulate properties of the zeolite crystals, „4th Solvenian-Croatian symposium on zeolites“, Ljubljana, Slovenia, October 18, 2011.
2. Topić Popović N (2011) Ichthyopathology Research at RBI, Croatia/Induction of Fish Cytochrome P450 Enzymes by Antibiotic Treatment, Texas A&M University, College of Veterinary Medicine & Biomedical Sciences, College Station, Texas, SAD, January 3, 2011.
3. Topić Popović N (2011) Consequences of the antimicrobials use in aquaculture to human health, 8th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, July 1, 2011.
4. Sauerborn Klobučar R (2011) Biomarkers/Biotests in environmental risk assessment, 8th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, July 1, 2011.
5. Barišić J (2011) Cultivation of freshwater fish in Israel, 8th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, July 1, 2011.

SELECTED ORGANIZED CONFERENCES AND MEETINGS

1. COST Domain Chemistry, Molecular Sciences & Technologies Action CM0603: „Free Radicals in Chemical Biology“, Final Scientific Meeting, Final Management Committee, Ruđer Bošković Institute, Zagreb, July 14-17, 2011 (Main organizer: Branka Mihaljević).
2. 8th Symposium of the Croatian Radiation Protection Association (with international participation), Krk, Croatia, April 13-15, 2011 (S. Miljanić and M. Ranogajec-Komor members of the Scientific Committee; Ž. Knežević member of the Organising Committee).
3. EURADOS WG9 Meeting, Zagreb, Croatia, October 24-25, 2011 (organised by S. Miljanić with contributions from Ž. Knežević and M. Majer).
4. Seminar „Irradiation methods in cultural heritage protection“, Zagreb, Croatia, October 4-5, 2011 (organized by Branka Katušin-Ražem and Mario Braun from Croatian Conservation Institute).
5. 8th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, July 1, 2011.
5. Perić B, Cordier S, Cuny J, Gautier R, Guizouarn T, Planinić, P. High-temperature experimental and theoretical study of magnetic interactions in diamond and pseudo-diamond frameworks built up from hexanuclear tantalum clusters. *Chem - Eur J* **17** (2011) 6263.
6. Fontaine B, Cordier S, Gautier R, Gulo F, Halet J-F, Perić B, Perrin C. Octahedral niobium cluster-based solid state halides and oxyhalides: effects of the cluster condensation via an oxygen ligand on electronic and magnetic properties. *New J Chem* **35** (2011) 2245.
7. Kosanović C, Falini G, Kralj D. Mineralization of Calcium Carbonates in Gelling Media. *Cryst Growth Des* **11** (2011) 269.
8. Mihaljević B, Tartaro I, Ferreri C, Chatgillaloglu C. Linoleic acid peroxidation vs. isomerization: a biomimetic model of free radical reactivity in the presence of thiols. *Org Biomol Chem* **9** (2011) 3541.
9. Čož-Rakovac R, Lisičić D, Šmuc T, Topić Popović N, Strunjak-Perović I, Jadan M, Tadić Z, Jug Dujaković J. Classification modelling of physiological stages in captive Balkan whip snakes using blood biochemistry parameters. *J Herpetol* **45** (2011) 525.
10. Ferri J, Topić Popović N, Čož-Rakovac R, Beer-Ljubić B, Strunjak-Perović I, Škeljo F, Jadan M, Petrić M, Barišić J, Šimpraga M, Stanić R. The effect of artificial feed on blood biochemistry profile and liver histology of wild saddled bream. *Oblada melanura* (Sparidae). *Mar Environ Res* **71** (2011) 218.
11. Kosanović C, Antonić Jelić T, Bronić J, Kralj D, Subotić B. Chemically controlled particulate properties of zeolites: towards the faceless particles of zeolite A. 1. Influence of the batch molar ratio $[\text{SiO}_2/\text{Al}_2\text{O}_3]_b$ on the size and shape of zeolite A crystals. *Micropor Mesopor Mat* **137** (2011) 72.

SELECTED PUBLICATIONS

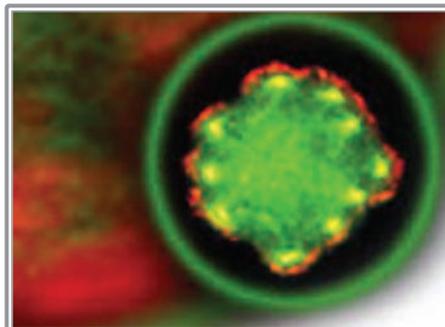
1. Gotić M, Dražić G, Musić S. Hydrothermal synthesis of $\alpha\text{-Fe}_2\text{O}_3$ nanorings with the help of divalent metal cations, Mn^{2+} , Cu^{2+} , Zn^{2+} and Ni^{2+} . *J Mol Struct* **993** (2011) 167.
2. Žic M, Ristić M, Musić S. Monitoring the hydrothermal precipitation of $\alpha\text{-Fe}_2\text{O}_3$ from concentrated $\text{Fe}(\text{NO}_3)_3$ solutions partially neutralized with NaOH, *J Mol Struct* **993** (2011) 115.
3. Palčić A, Bronić J, Brlek Đ, Subotić B. New insights on the autocatalytic nucleation in zeolite A synthesis. *CrystEngComm*, **13** (2011) 1215.
4. Miletić G, Blažina Ž. Theoretical study of magnetism in RM12B6 compounds (R=Y, La or Ce, M= Fe, Co). *J Magn Magn Mater* **323** (2011) 2340.

DIVISIONAL ORGANISATION

Head: Igor Weber

The Division of Molecular Biology consists of the following laboratories:

- ⇒ Laboratory for Molecular Genetics, Dušica Vujaklija
- ⇒ Laboratory of Chemical Biology, Branka Salopek Sondi
- ⇒ Laboratory of Molecular Microbiology, Davor Zahradka
- ⇒ Laboratory of Neurochemistry and Molecular Neurobiology, Lipa Čičin-Šain
- ⇒ Laboratory of Molecular and Cell Biology, Ivica Rubelj
- ⇒ Laboratory for Genotoxic Agents, Maja Osmak
- ⇒ Laboratory for Structure and Function of Heterochromatin, Miroslav Plohl
- ⇒ Laboratory for Evolutionary Genetics, Đurđica Ugarković
- ⇒ Laboratory for Electron Microscopy, Hrvoje Fulgosi



expertise and application of acquired knowledge, methodologies and skills to the broader community. Research areas in the Division are focused on exploring different aspects of molecular and cellular biology studied in microbial, animal and plant organisms. The particular goals of the research program are to explore non-coding repetitive sequences in genome structuring; to study structures and processes at telomeres; to study processes essential for maintaining genome integrity, plasticity and evolution; to decipher evolutionary patterns of conserved genes and appearance of new genes; to characterize general and specific transcription factors and their mechanisms of action; to study how cells communicate, differentiate, move and adhere; to investigate molecular mechanisms involved in cell response to genotoxic compounds; to examine the potential of genetically targeted adenoviruses; to explore photosynthesis; and to study regulation of plant growth and development, as well as the function of plant secondary metabolites.

OVERVIEW OF THE DIVISION

The mission of the Division of Molecular Biology is to advance our knowledge on fundamental biological questions by conducting high-quality, internationally recognized knowledge-driven scientific research on major topics in contemporary biology, from molecules to cells and organisms. We also participate in the transfer of knowledge by contributing to education, and by offering

TOP ACHIEVEMENTS

Sponge non-metastatic Group I

Nme gene/protein - structure and function is conserved from sponges to humans

The objective of this study was primarily to determine the structure and biochemical characteristics of the sponge NmeGp1Sd in order to gain a deeper insight into the evolution of metazoan Nme proteins and their functions. Our results suggest that the ancestor of all animals possessed NmeGp1 with properties and functions similar to the evolutionarily recent versions of the protein even before the appearance of true tissues and origin of tumors and metastasis (Perina et al., 2011).



Fig. 1. Marine sponge *Suberites domuncula* in symbiosis with hermit crab.

Late activation of stress-activated protein kinases/C-JUN-N-terminal kinases triggered by cisplatin-induced DNA damage repair defective cells.

The data presented in this paper indicate that late SAPK/JNK activation is triggered by non-repaired cisplatin adducts in transcribed genes and involves replication-associated events, DSBs, tyrosine kinases, Rho GTPases, and specific repair factors (Helbig et al., 2011).

A novel telomeric sequence in insects

The TTAGG repeat is generally reputed to be the canonical telomeric motif within the class Insecta. By studying telomeric DNAs in 30 coleopteran beetles, we showed that arrays built of a TCAGG repeat substitute for (TTAGG) $_n$ sequences in all tested species within the superfamily Tenebrionoidea. Our results therefore confirm (TCAGG) $_n$ repeats as the first sequence-motif alternative to TTAGG-type chromosome ends in insects (Mravinac et al., 2011).

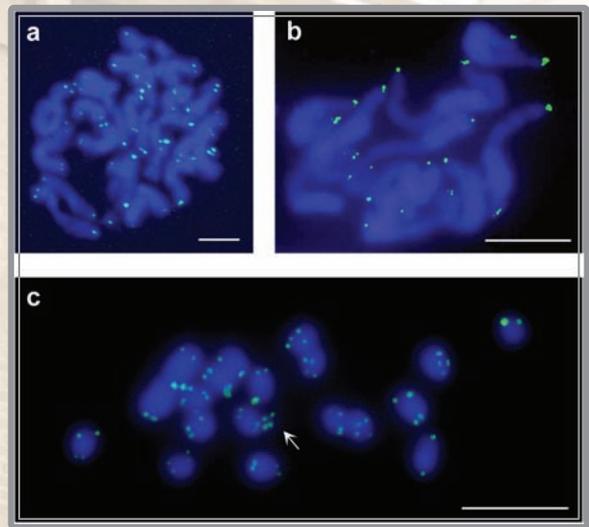


Fig. 2. Distribution of TTAGG (a) and TCAGG repeats (b and c) at chromosome ends of insect species *Chrysolina americana* (a), *Tenebrio molitor* (b), and *Tribolium castaneum* (c). Chromosome spreads are counterstained with DAPI (blue), while green signals correspond to telomeric sequences. Scale bars, 5 μ m.

Subcellular distribution of glutathione and its dynamic changes under oxidative stress in the yeast *Saccharomyces cerevisiae*

The subcellular distribution of glutathione was studied in *Saccharomyces cerevisiae* by quantitative immunoelectron microscopy. The highest glutathione content was detected in mitochondria and subsequently in the cytosol, nuclei, cell walls, and vacuoles.

The induction of oxidative stress by hydrogen peroxide (H₂O₂) led to changes in glutathione-specific labeling. Additionally, large amounts of glutathione were relocated and stored in vacuoles in cell type III, suggesting the importance of the sequestration of glutathione in vacuoles under oxidative stress (Zechmann et al., 2011).

Development of hydrocephalus and classical hypothesis of cerebrospinal fluid hydrodynamics: facts and illusions

Based on our experimental results and our new hypothesis of cerebrospinal fluid (CSF) physiology we have abandoned the circulation (“classic”) hypothesis of hydrocephalus development and have proposed a new working hypothesis for hydrocephalus etiopathology. Thus, changes in the interstitial-cerebrospinal fluid functional unit should be included in the pathophysiology of fluid accumulation inside the CSF system. We presume that all pathological processes in which an increase of CSF osmolarity or CSF pressure takes place could result in hydrocephalus development without significant obstruction or stenosis (circulation hypothesis) of the CSF system (Orešković & Klarica, 2011).

Genes are spontaneously created

Evidence is presented that, in addition to copying, spontaneous (de novo) creation of completely new genes has an important role in the evolution of genomes. For these orphan genes, which play an important role in embryonic development and the interaction of organisms with the environment, the authors have demonstrated that they can originate at any time during evolution, which also includes the organisms currently living on earth (Tautz & Domazet-Lošo, 2011).

Serotonin level and serotonin uptake in human platelets: a variable interrelation under marked physiological influences

Platelet serotonin (5HT) system is often studied as a potential indicator of serotonin dysregulation in various disease conditions. We have shown an unexpectedly low correlation between two directly related platelet serotonin parameters: granular 5HT level and velocity of membrane 5HT uptake, which argues against the use of platelet 5HT level as an indirect measure of platelet 5HT transporter activity in humans, and also against its use as peripheral measure of neuronal 5HT transporter functionality. These results also implicate gender and seasonality as important in peripheral serotonergic mechanisms (Balija et al., 2011).

EDUCATION

In 2011, members of the Division of molecular biology participated in the teaching of more than 15 undergraduate and graduate courses and more than 20 postgraduate courses at the Universities in Zagreb, Split, Dubrovnik and Osijek. During this year they also supervised more than 15 diploma, MSc, and PhD theses. A series of practical courses in biology and medicine was organized in our Division by Andreja Ambriović Ristov (<http://www.tecajevi-irb.com>).

AWARDS

Darko Orešković received the Annual RBI award for 2011. awarded for publishing a scientific paper in a high impact factor journal in the field of molecular biology.

Hrvoje Fulgosi received the Annual RBI award for 2011. awarded for a research project funded by International Center for Genetic Engineering and Biotechnology (ICGEB).



Fig. 3. Fetus day 14 and day 18. Size compared to 5 croatian lipas.

PROJECTS

Program supported by the Ministry of Science, Education and Sport

1. Molecular fundamentals of biological processes, Miroslav Plohl.

Projects supported by the Ministry of Science, Education and Sport

1. Increase of adenovirus transduction efficacy and resistance to cytostatics, Andreja Ambriović Ristov
2. Serotonergic transmission: genes, proteins and behavior, Jasminka Štefulj
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: structure, function and evolution, 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
18. Genetic studies of BPC-157 effect on micro-organisms, Senka Džidić

Research, developmental and international projects

1. Isolation and characterization of bioactive metabolites from medicinal plants grown in the greenhouse and *in vitro* by plant tissue culture, Dunja Šamec (National Croatian Science Foundation)
2. Expression of a *KCS* gene from *Cardamine graeca* in *Cucurbita pepo* to engineer nervonic acid-enriched seed oils, Snježana Mihaljević (Croatian Academy of Sciences and Arts – HAZU)
3. Molecular characterization of cyanobacterial system suitable for biological production of hydrogen, Hrvoje Fulgosi (Croatian Academy of Sciences and Arts - HAZU)
4. Identification of bioactive metabolites in medicinal plants and their *in vitro* propagation, Dunja Šamec (UKF Gaining Experience Grant 2A)
5. Exploring and exploiting the bacterial diversity in the West Istria Sea: focus on marine actinomycetes, Dušica Vujaklija (MSES, COGITO-bilateral project with France, 910-08/10-01/00072)
6. Control of plant growth and senescence by energetic status of chloroplasts, Hrvoje Fulgosi (MSES, bilateral project with Germany, 910-08/10-01/00192)
7. Diaryrtriazens: a new group of potential anticancer drugs, Anamaria Brozović (MSES,

- bilateral project with Slovenia, 910-08/08-01/00312)
8. Vectors for precise targeting into unique genomic loci, Ivica Rubelj (Croatian Institute of Technology)
 9. EpiGeneSys, WP4: Signalling to the Epigenome, Đurđica Ugarković (EC FP7 Network of Excellence)
 10. Epigenetics: Bench to Bedside, Đurđica Ugarković (COST Action TD0905)
 11. Metagenomic analysis of environmental microbial communities in marine sediments, Dušica Vujaklija (Adris Group Donation, 03-7466/2-2011)



Fig. 4. Testing of strength of Wistar Zagreb-5HT rat in the string test.

SELECTED INVITED LECTURES

1. Vujaklija D: Streptomycetes are a source of hydrolytic enzymes with potential in lipid biotransformation. CIPKEBIP Annual Conference: "Biosynthetic and metabolic Engineering in Industrial drug and process de-

- velopment". Ljubljana, Slovenia, September 15-16, 2011.
2. Pleše B, Četković H: Sponges: simple animals with complex genomes. Memorias XLVI Congreso Nacional de Ciencias Biologicas. Medellin, Colombia, October 10-15, 2011.
3. Meštrovic N, Castagnone-Sereno P, Plohl M: Origins and evolution of satellite DNAs: the nematode view. 63rd International Symposium on Crop Protection. Ghent University, Belgium, May 23-25, 2011.
4. Fulgosi H, Vojta L, Jurić S, Tomašić Paić A: Final step in energy conductance from thylakoid complexes to stromal reducing equivalents as a source of metabolic retrograde signals. Plant Organellar Signaling from Algae to Higher Plants. Primošten, Croatia, August 31 – September 3, 2011.
5. Bruvo B, Pezer Ž, Pons J, Ugarković Đ: Phylogeny of Coleoptera: Development of New Molecular Markers. 5th Dresden Meeting on Insect Phylogeny. Dresden, Germany, September 23-25, 2011.

SELECTED ORGANIZED CONFERENCES

1. Young scientist meeting at RBI - ZS3V, Zagreb, Croatia, July 7-8, 2011 (D. Vujaklija)
2. Workshop "COST Action TD0905 Epigenetics-Bench to Bedside", Split, Croatia, April 28-30, 2011 (Đ. Ugarković)

SELECTED PUBLICATIONS

Review articles

1. Tautz D, Domazet-Lošo T. The evolutionary origin of orphan genes. *Nat Rev Genet* **12** (2011) 692.
2. Orešković D, Klarica M. Development of hydrocephalus and classical hypothesis of cerebrospinal fluid hydrodynamics: facts and illusions. *Prog Neurobiol* **94** (2011) 238.

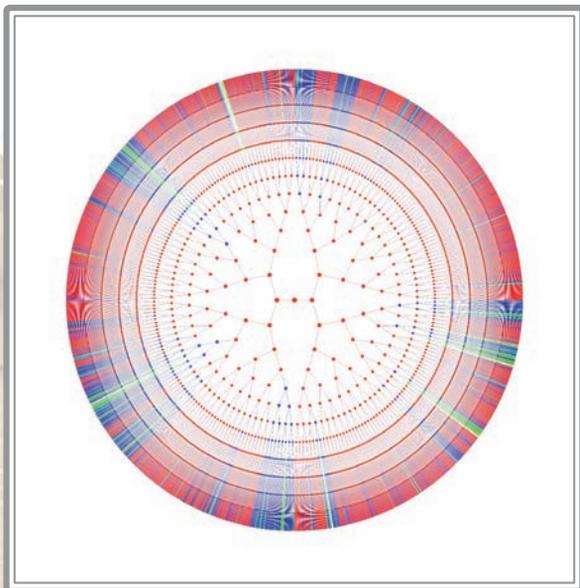


Fig. 5. Schematic presentation of cell growth heterogeneity created by abrupt telomere shortening. Each circle represent one round of cell divisions. Red - telomeres undergo gradual shortening; blue - one abrupt shortening; green - two abrupt shortening; white - three abrupt shortenings.

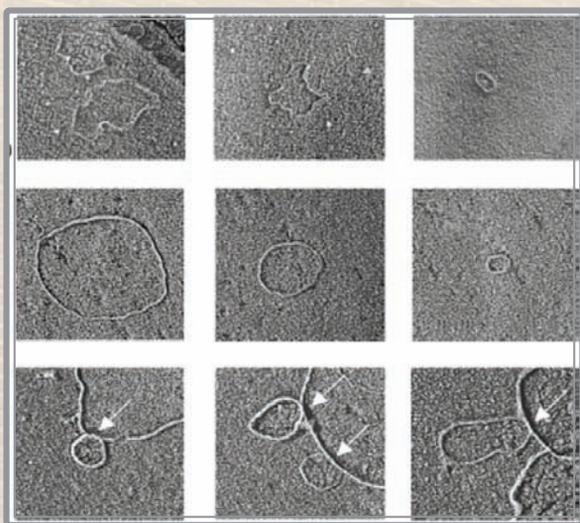


Fig. 6. Abrupt telomere shortening in normal human cells. Extrachromosomal telomeric DNA circles from MJ90 cells and NF cells. EM images are shown in reverse contrast.

Additional publications

1. Mravinac B, Meštrović N, Čavrak VV, Plohl M., TCAGG, an alternative telomeric sequence in insects. *Chromosoma (Berlin)* **120** (2011) 367.
2. Perina D, Herak Bosnar M, Bago R, Mikoč A,

Harcet M, Deželjin M, Četković H. Sponge non-metastatic Group I Nme gene/protein - structure and function is conserved from sponges to humans. *BMC Evol Biol* **11** (2011) 87.

3. Helbig L, Damrot J, Hülsenbeck J, Köberle B, Brozović A, Osmak M, Fiket Ž, Kaina B, Fritz G. Late activation of stress-activated protein kinases/C-JUN-N-terminal kinases triggered by cisplatin-induced DNA damage repair defective cells. *J Biol Chem* **286** (2011) 12991.
4. Annesley SJ, Bago R, Herak Bosnar M, Filić V, Marinović M, Weber I, Mehta A, Fisher PR. *Dictyostelium discoideum* nucleoside diphosphate kinase C plays a negative regulatory role in phagocytosis, macropinocytosis and exocytosis. *PLoS One* **6** (2011) e26024-1.
5. Perina D, Herak Bosnar M, Mikoč A, Četković H. Characterization of Nme6-like gene/protein from marine sponge *Suberites domuncula*. *Naunyn Schmiedebergs Arch Pharmacol* **384** (2011) 451.
6. Bališa M, Bordukalo-Nikišić T, Mokrović G, Banović M, Čičin-Šain L, Jernej B. Serotonin level and serotonin uptake in human platelets: a variable interrelation under marked physiological influences. *Clin Chim Acta* **412** (2011) 299.
7. Supek F, Šumanovac Ramljak T, Marjanović M, Buljubašić M, Kragol G, Ilić N, Šmuc T, Zahradka D, Mlinarić-Majerski K, Kralj M. Could LogP be a principal determinant of biological activity in 18-crown-6 ethers? Synthesis of biologically active adamantane-substituted diaza-crowns. *Eur J Med Chem* **46** (2011) 3444.
8. Čimbora-Zovko T, Brozović A, Piantanida I, Fritz G, Virag A, Alič B, Majce V, Kočevar M, Polanc S, Osmak M. Synthesis and biological evaluation of 4-nitro-substituted 1,3-diaryltriazenes as a novel class of potent antitumor agents. *Eur J Med Chem* **46** (2011) 2971.
9. Mihaljević S, Radić S, Bauer N, Garić R, Mihaljević B, Horvat G, Leljак-Levanić D, Jelaska S. Ammonium-related metabolic changes affect somatic embryogenesis in pumpkin (*Cucurbita pepo* L.). *J Plant Physiol* **168** (2011) 1943.
10. Piljac-Žegarac J, Šamec D. Antioxidant stability of small fruits in postharvest storage at

room and refrigerator temperatures. *Food Res Int* **44** (2011) 345.

11. Zechmann B, Liou L-C, Koffler BE, Horvat L, Tomašić Paić A, Fulgosi H, Zhang Z. Subcellular distribution of glutathione and its dynamic changes under oxidative stress in the yeast *Saccharomyces cerevisiae*. *FEMS Yeast Res* **11** (2011) 631.

BOOKS

1. Ugarković Đ (editor) Long Non-Coding RNAs. *Prog Mol Subcell Biol*, Vol. 51, Springer Verlag Heidelberg, 2011.
2. Acute Leukemia - The Scientist's Perspective and Challenge, Antica M (ed.), InTech, 2011.

CHAPTERS IN BOOKS

1. Weber I. Interference Reflection Microscopy. In: *Encyclopedia of Life Sciences (ELS)*, Zheng Y (ed.), John Wiley & Sons, 2011.
2. Pezer Ž, Brajković J, Feliciello I, Ugarković Đ. Transcription of satellite DNAs in Insects. In: *Long Non-Coding RNAs*, Ugarković Đ (ed.), *Prog Mol Subcell Biol* 51: 161-179, Springer Verlag, 2011.
3. Antica M. Lymphocyte Commitment and Ikaros Transcription Factors. In: *Acute Leukemia - The Scientist's Perspective and Challenge*, Antica M (ed.), InTech, 2011.

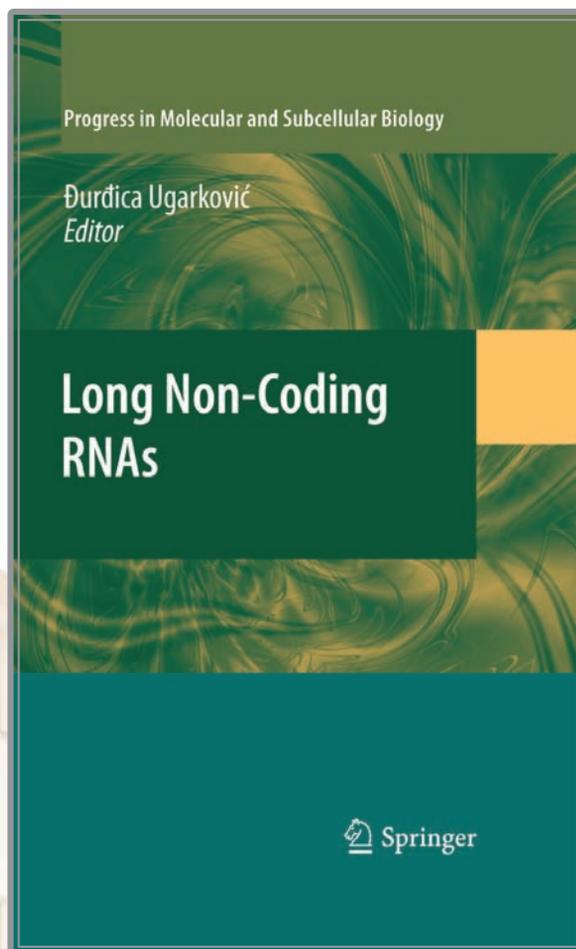


Fig. 7. This book reviews the rapidly advancing field of long ncRNAs describing the epigenetic and non-epigenetic mechanisms by which they regulate various biological functions in model systems, from yeast to mammals.



DIVISIONAL ORGANIZATION

Head: Đurđica Ugarković

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

- ⇒ Laboratory for Systems Biomedicine, Mario Cindrić
- ⇒ Laboratory of Experimental Hematology, Immunology and Oncology, Jelka Gabrilovac
- ⇒ Laboratory of Molecular Virology and Bacteriology, Magdalena Grce
- ⇒ Laboratory of Molecular Endocrinology and Transplantation, Mirko Hadžija
- ⇒ Laboratory of Experimental Therapy, Marijeta Kralj
- ⇒ Laboratory for Reactive Radicals, Tatjana Marotti
- ⇒ Laboratory of Molecular Neuropsychiatry, Dorotea Mück-Šeler
- ⇒ Laboratory of Molecular Oncology, Jasminka Pavelić
- ⇒ Laboratory for Epigenomics, Koraljka Gall Trošelj
- ⇒ Laboratory of Molecular Neuropharmacology, Silva Katušić Hećimović
- ⇒ Group for Translation Medicine, Oliver Vugrek
- ⇒ Laboratory for Oxidative Stress, Neven Žarković
- ⇒ Laboratory for Hereditary Cancer, Sonja Levanat
- ⇒ Laboratory for Personalized Medicine, Sanja Kapitanović
- ⇒ Animal Facility Unit, Ranko Stojković



OVERVIEW OF THE DIVISION

The mission of the Division of Molecular Medicine (DMM) is closely correlated with major areas of human medicine, covering a broad spectrum of research topics reflected in the names of its laboratories. The majority of research topics are oriented towards molecular aspects of cancer, neuroscience (neuropsychiatry, neurodegeneration, neuropharmacology), stress-related diseases and their models. Particular attention and research has been devoted to the mechanisms of disease etiology arising from disturbed methylation of macromolecules (DNA/proteins), molecular mechanisms of disease etiopathogenesis and experimental therapies. The DMM, with its Human Tumor Bank and numerous clinical samples collected through collaborations with clinicians (e.g. in neuropsychiatry and neurodegeneration), represents an important biomedical core, dedicated to establishing and refining new strategies and methods for understanding the molecular mechanisms of disease, for improving diagnostic procedures and therapies and, of primary importance, for disease prevention.

TOP ACHIEVEMENTS

Biomarkers of ADHD and/or treatment response in depressed patients

We have shown that an increase in relative levels of biantennary glycans with antennary fucose, and a decrease in branching of plasma glycans is found in children with ADHD compared to control children (Pivac et al., 2011a). This work suggests that there is potential for the use of the plasma N-glycome as biomarkers for ADHD. Furthermore, we find that the basal lipid profile might be used as a biomarker for treatment response to paroxetine in depressed patients (Muck-Šeler et al., 2011).

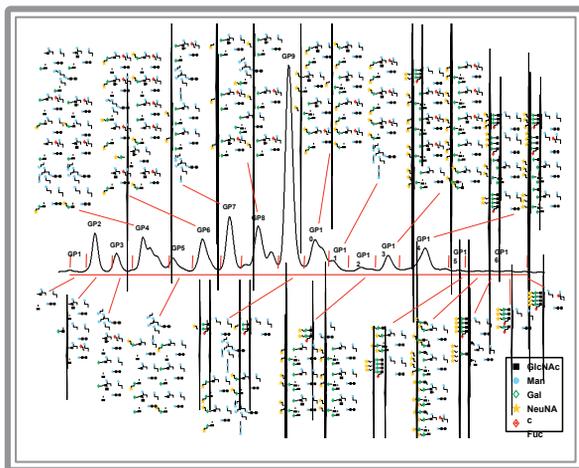


Figure 1. Composition of the plasma N-glycome (GlcNAc – N-acetylglucosamine; Man – mannose; Gal – galactose; NeuNAc – N-acetylneuraminic acid (sialic acid); Fuc – fucose)

Genetic markers of suicidal behaviour or psychosis

In female suicide victims the presence of one or two Met alleles of the brain derived neurotrophic factor (BDNF Val66Met) was associated with suicide, especially violent suicide, suggesting that the BDNF66Met allele might be a risk factor for suicide (Pregelj et al., 2011). In male patients with Alzheimer's disease, the presence of the BDNF 66Met allele was associated with psychotic symp-

toms (Pivac et al., 2011c). In male control subjects compared to male suicide victims, the overpresentation of the Met/Met genotype in the catechol-O-methyltransferase (COMT Val108/158Met) was detected. These results indicate that this genotype might be a protective factor against suicide (Pivac et al., 2011b). In contrast to the findings obtained in suicide victims, suicidal attempts were significantly associated with the COMT Met/Met genotype in male alcoholic subjects (Nedić et al., 2011).

A new method for nonlinear spectral image segmentation

A new method for nonlinear spectral image segmentation of histologic samples without use of contrast was developed which is equivalent to methods using contrast agents, or coloring (Kopriva et al., 2011).

Reconsideration of anticancer immunotherapy by poly (I:C) usage

Poly (I:C) usage in anticancer immunotherapy needs to be reevaluated as it was found that this kind of therapy may cause tumor progression and invasiveness (Matijević and Pavelić, 2011).

Novel potential anticancer compounds

In 2011 over 150 newly synthesized compounds were screened in vitro for potential antitumor activity. Studies of the potential antitumor ability of crown ether compounds, together with the search for structural features that influence antiproliferative activity in a diverse set of 19 known oxa-, monoaza- and diaza-18-crown-6 ethers, using nonlinear Support Vector Machines regression, clearly showed that relying primarily on the logP is a sensible strategy in preparing future 18-crown-6 analogs with optimized biological activity (Supek et al., 2011).

TP53 mutational signature for aristolochic acid as a causative agent in endemic nephropathy

Unique TP53 mutations, A:T to T:A conversions localized on the non-transcribed strand of the p53 gene, were identified in endemic nephropathy patients, supporting the hypotheses that botanical products containing aristolochic acid, a carcinogen and nephrotoxin, are responsible, in part, for the high prevalence of upper urinary tract carcinoma and chronic renal disease in countries where Aristolochia herbal remedies traditionally have been used for medicinal purposes (Masaaki et al., 2011).

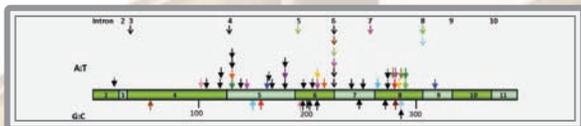


Figure 2. The locations of mutations in the TP53 gene in patients with endemic nephropathy/upper urinary tract carcinoma

A new function of APN/CD13 in MR-mediated phagocytosis

The involvement of aminopeptidase N (APN; CD13) in FcγR-independent phagocytosis, which is mediated *via* mannose receptors (MR) was studied in J774 cells which originate from murine macrophages. APN/CD13 expressed on J774 cells co-localize with the MR, and co-internalize upon MR ligation by ovalbumin, thus showing a new function of APN/CD13 in MR-mediated phagocytosis (Gabrilovac et al., 2011).

Collaborative studies of the Nme metastasis suppressor in model organisms

Collaborative studies on the Group I Nme gene/protein reveal that human Nme1 and Nme2 and the single sponge Nme Group I homolog share several structural and biochemical characteristics which suggests that the ancestral Group I Nme gene/protein was

probably very similar to the present day multifunctional enzyme. Since the sponge Nme Group I homolog suppresses migration in human cells it is presumed that migration, essential for metastasis formation, is an evolutionarily very old process (Perina et al., 2011). Studies in *Dictyostelium discoideum* reveal that one of the Nme variants in this model organism (NDPK-C) negatively regulates endocytosis which is opposite to its positive role in higher eukaryotes (Annesley et al., 2011).

HNE-protein adducts in C. Kessleri as a sign of environmental pollution

The discovery of an increase of 4-hydroxy-2-nonenal (HNE) in the green algae *C. Kessleri* upon herbicide exposure strongly points out the need for evaluation of HNE-protein adducts in *C. Kessleri* as a sign of environmental pollution and, as such, should be added to standard toxicity tests (Špoljarić et al., 2011).

NEW EQUIPMENT

1. High resolution microarray scanner
2. Microarray spotter robot
3. Bioanalyzer (IPA project)
4. PCR machine (IPA project)
5. -80 C freezer (IPA project)

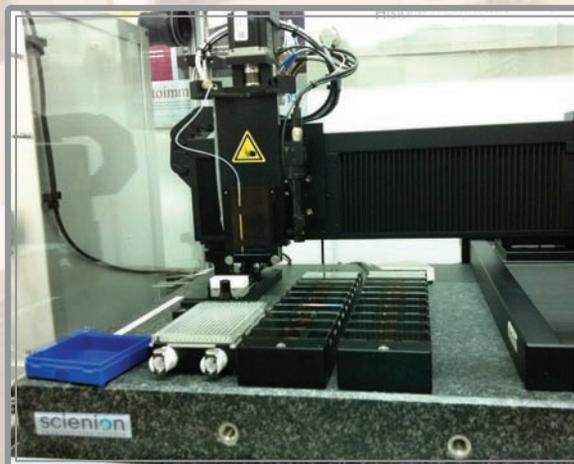


Figure 3. Microarray Spotter Robot



Figure 4. Bioanalyzer

EDUCATION

Researchers in the DMM are active in education at different universities, as principal teachers, organizing and actively participating in various bachelor's, master's and doctoral courses.

PROGRAMS AND PROJECTS

Programs supported by the Ministry of Sciences, Education and Sports

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

Projects supported by the Ministry of Sciences, Education and Sports

1. Cytochrome P450 monooxygenase and tumor appearance in ageing and oxidative stress, Tatjana Marotti
2. Gene therapy of tumors by modulating the molecules of the immune system, Jasminka Pavelić
3. The role of nm23 genes in oral squamous cell carcinoma, Maja Herak Bosnar

4. The role of p53/p73 network in soft tissue sarcoma, Neda Slade
5. The mechanism of cholesterol action in the pathogenesis of Alzheimer's disease, Silva Katušić Hećimović
6. Stress, GABA-A receptors and mechanisms of action of neurophychoactive drugs, Dubravka Švob Štrac
7. The role of different cell death responses to DNA-damage treatment, Marijeta Kralj
8. S-Adenosylhomocysteine hydrolase (AHCY) deficiency: Molecular mechanisms of a new human disease, Oliver Vugrek
9. Role of membrane peptidases on tumor and normal cells, Jelka Gabrilovac
10. Signal transduction in tumors: Hh-Gli interactions and therapeutic potential, Sonja Levnat
11. Pharmacogenomics and proteomics of serotonergic and catecholaminergic system, Dorotea Muck-Šeler
12. Molecular basis and treatment of psychiatric and stress related disorders, Nela Pivac
13. Lipids, free radicals and their second messengers in integrative oncology, Neven Žarković
14. Molecular genetics and pharmacogenetics of gastrointestinal tumors, Sanja Kapitanović
15. Proteomic prostate tumor biomarker analysis, Mario Cindrić
16. Obtaining the structures like Langherhans islets from mouse stem cells, Mirko Hadžija
17. Aberrant DNA methylation in HPV associated lesions, Magdalena Grce
18. Epigenetic and immunomodulatory changes in malignant head and neck tumours, Koraljka Gall Trošelj

Additional projects at the DMM:

1. New therapeutic modalities in treatment of malignant diseases, Marko Radačić
2. Genetic basis in development of pituitary tumors, Živko Gnjidić
3. Pharmacogenetics in pediatric oncology, Jasenka Stepan Giljević
4. Eye immunology, Iva Dekaris

5. Molecular basis of aseptic instability of hip total endoprothesis, Robert Kolundžić

Research development and international projects

Billateral Projects:

1. Alzheimer disease – the role of cholesterol on processing and localization of APP protein family, Silva Katušić Hećimović (Croatia-Germany)
2. The development of new approaches for molecular and serological diagnostic of human papillomavirus (HPV) infection, Magdalena Grce (Croatia France)
3. Improvements of adhesive properties of biomedical materials by plasma treatment, Morana Jaganjac (Croatia-Slovenia)
4. Molecular dynamic S-adenozylhomocystein hidrolasys (SAHH) and its role in gene expression, Oliver Vugrek (Croatia-Israel)

The Instrument for Pre-Accession Assistance - IPA

Creation of research related infrastructure for Translational Medicine and Applied Genomics, Oliver Vugrek

BICRO

The synthesis of disulphoxy and three sulphony analogs for identification of peptides and proteins by mass spectrometry, Mario Cindrić

COST Project

Action CM1103: Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain, Dorotea Mück-Šeler, Nela Pivac

Croatian Science Foundation

Detection and tracking of biological markers for

early therapeutic intervention in sporadic Alzheimer's disease. Collaborators: Nela Pivac, Dorotea Mück-Šeler, Maja Mustapić, Matea Nikolac, Gordana Nedić, Dubravka Švob Štrac, Maja Jazvinščak Jembrek.

SELECTED LECTURES

1. Katušić Hećimović S. Endocytic traffick jam in Niemann Pick type C disease – a cause of increased Alzheimer's amyloid- β peptide formation, Gordon Research Conference – Lysosomal Diseases, Galveston, TX, SAD, January 23-28, 2011.
2. Katušić Hećimović S. The molecular mechanism(s) of increased amyloid-beta peptide in Niemann-Pick type C disease, Sahlgren University Hospital, Neurochem Laboratory, Mölndal, Sweden, March 18, 2011.
3. Katušić Hećimović S. The molecular mechanism(s) of increased Abeta upon cholesterol accumulation in Niemann-Pick type C disease, Deutsches Zentrum für Neurodegenerative Erkrankungen (DZNE) & Adolf Butenandt-Institute, Biochemistry, Ludwig-Maximilians-University, Munich, Germany, June 10, 2011.
4. Pivac N. Molecular mechanisms in traumatic brain injury. „Wounds of war III: coping with blast related traumatic brain injury in returning troops“ NATO advanced research workshop. Vienna, Austria, February 20-22, 2011.
5. Pivac N. Nedić G, Nikolac M, Fistonić M, Kovačević M, Mustapić M, Gverić Korkut I, Grubišić-Ilić M, Kozarić-Kovačić D, Mück-Šeler D. Neurobiological Basis of Pain Syndrome in War Veterans with PTSD: Preliminary Findings. „Wounds of war IV: Pain syndromes - from recruitment to returning troup.“ NATO Advanced Research Workshop. Klopeiner See, St Kantian, Austria, September 9 – October 2, 2011.
6. Ozretić P. *In silico* methods for assessing potential functional impact of human breast cancer gene BRCA2 sequence variants found in 5' untranslated region “16th World Congress on Advances in Oncology and 14th

- International Symposium on Molecular Medicine, Rhodes, Greece, October 6-8, 2011.
7. Gall Trošelj K. Curcumin and resveratrol influence the balance between EZH2 and JMJD3 in cancer cell lines in vitro, ICMAN 5 - The Fifth International Conference on Mechanisms of Action of Nutraceuticals, Brisbane, Australia, October 13-15, 2011.
 8. Jaganjac M. Lipid peroxidation – a missing link in tumor regression. Analytical methods to study oxidative damage, antioxidants and drugs. Białystok, Poland, November 10-13, 2011
 9. Jaganjac M. Lipid peroxidation – environmental causes and the role in tumor development. Biomedical Engineering Sciences, Environmental Management and Ecotoxicology at University of Applied Sciences Technikum Wien, Austria, November 25, 2011
 10. Čipak Gašparović A. PUFA producing yeast –model for adaptation to membrane changes based on oxidative stress. Analytical methods to study oxidative damage, antioxidants and drugs. Białystok, Poland, November 10-13, 2011
 11. Levanat S. Molecular mechanisms of skin diseases. 22nd Ljudevit Jurak International Symposium on Comparative Pathology, Zagreb, Multimedia center Sestre Milosrdnice Clinical Hospital Centre, Zagreb, June 3 - 4, 2011.
 12. Levanat S. Translational research in molecular biology of breast cancer-new achievements and clinical application. 21st Scientific meeting on Breast Diseases, Croatian Academy of Sciences and Arts, HAZU, Zagreb, September 15, 2011.
 13. Levanat S. Molecular genetics in clinical breast cancer treatment. Celebration of 45 the years of Croatian Ligue Against Cancer, dedicated to Breast cancer «Love your breast», Croatian Medical Association, Zagreb, October 22, 2011.
 14. Levanat S. Predictive diagnosis of breast cancer/2nd Croatian Symposium in Predictive Medicine with Internacional Participation. Role of Laboratory medicine in predictive medicine: Cancer diseases. Zagreb, November 4, 2011.
 15. Slade N, Brdar B, Jelaković B, Moriya M, Medverec Z, Tomić K, Karanović S, Vuković Lela I, Fernandes A, Wu L, Grollman AP. TP53 mutational signature of aristolochic acid in carcinomas of the upper urinary tract. 44th Annual Scientific Meeting of the European Society for Paediatric Nephrology. Cavtat, Croatia, September 14-17, 2011.

SELECTED PUBLICATIONS

Selected research articles

1. Pivac N, Knežević A, Gornik O, Pučić M, Igl W, Peeters H, Crepel A, Steyaert J, Novokmet M, Redžić I, Nikolac M, Novković Hercigonja V, Dodig Ćurković K, Ćurković M, Nedić G, Muck-Šeler D, Borovecki F, Rudan I, Lauc G. Human plasma glycome in attention-deficit hyperactivity disorder and autism spectrum disorders. *Mol Cell Proteomics* **10.1** (2011a) 1.
2. Shah AA, Leidinger P, Keller A, Wendschlag A, Backes C, Baus Lončar M, Meese E, Blin N. The intestinal factor Tff3 and a miRNA network regulate murine caloric metabolism. *RNA biology* **8** (2011) 77.
3. Kopriva I, Hadžija M, Popović Hadžija M, Korolija M, Cichočki A. Rational Variety Mapping for Contrast-Enhanced Nonlinear Unsupervised Segmentation of Multispectral Images of Unstained Specimen. *Am J Pathol* **179** (2011) 547.
4. Stepanić V, Koštrun S, Malnar I, Hlevnjak M, Butković K, Čaleta I, Dukši M, Kragol G, Makaruha-Stegić O, Mikac L, Ralić J, Tatić I, Tavčar B, Valko K, Zulfikari S, Munić V. Modeling Cellular Pharmacokinetics of 14- and 15-membered Macrolides with Physicochemical Properties. *J Med Chem* **54** (2011) 719.
5. Moriya M, Slade N, Brdar B, Medverec Z, Tomić K, Jelaković B, Wu L, Truong S, Fernandes A, Grollman AP. TP53 Mutational signature for aristolochic acid: an environmental carcinogen. *Int J Cancer* **129** (2011) 1532.
6. Muck-Šeler D, Šagud M, Mihaljević-Peleš A, Jakovljević M, Pivac N. Baseline lipid levels

- and acute treatment response to paroxetine and tianeptine in depressed women. Letters to the Editors. *J Clin Psychopharmacol* **31** (2011) 387.
7. Nedić G, Nikolac M, Nenadić Šviglin K, Mück-Šeler D, Borovečki F, Pivac N. Association study of a functional catechol-O-methyltransferase (COMT) Val108/158Met polymorphism and suicide attempts in patients with alcohol dependence. *Int J Neuropsychopharmacol* **14** (2011) 377.
 8. Annesley SJ, Bago R, Herak Bosnar M, Filić V, Marinović M, Weber I, Mehta A, Fisher PR. Dictyostelium discoideum nucleoside diphosphate kinase C plays a negative regulatory role in phagocytosis, macropinocytosis and exocytosis. *PLoS One* **6** (2011) e26024-1. pitati u ciji zavod
 9. Gabrilovac J, Čupić B, Živković E, Horvat L, Majhen D. Expression, regulation and functional activities of aminopeptidase N (EC 3.4.11.2 ; APN ; CD13) on murine macrophage J774 cell line. *Immunobiology* **216** (2011), 132.
 10. Matijević T, Pavelić J. The dual role of TLR3 in metastatic cell line. *Clin Exp Metastasis* **28** (2011) 701.
 11. Pivac N, Pregelj P, Nikolac M, Zupanc T, Nedić G, Mück-Šeler D, Videtić Paska A. The association between catechol-O-methyl-transferase Val108/158Met polymorphism and suicide. *Genes, Brain Behav* **10** (2011b) 565.
 12. Pregelj P, Nedic G, Videtić Paska A, Zupanc T, Nikolac M, Balažić J, Tomori M, Komel R, Muck-Šeler D, Pivac N. The association between brain-derived neurotrophic factor polymorphism (BDNF Val66Met) and suicide. *J Affect Disord* **128** (2011) 287.
 13. Perina D, Herak Bosnar M, Bago R, Mikoč A, Harcet M, Deželjin M, Četković H. Sponge non-metastatic Group I Nme gene/protein - structure and function is conserved from sponges to humans. *BMC Evolut Biol* **11** (2011) 87e.
 14. Špoljarić D, Čipak A, Horvatić J, Andrišić L, Waeg G, Žarković N, Jaganjac M. Endogenous 4-hydroxy-2-nonenal in microalga *Chlorella kessleri* acts as a bioactive indicator of pollution with common herbicides and growth regulating factor of hormesis. *Aquat Toxicol* **105** (2011) 552.
 15. Supek F, Šumanovac Ramljak T, Marjanović M, Buljubašić M, Kragol G, Ilić N, Šmuc T, Zahradka D, Mlinarić-Majerski K, Kralj M. Could LogP be a principal determinant of biological activity in 18-crown-6 ethers? Synthesis of biologically active adamantane-substituted diaza-crowns. *Eur J Med Chem* **46** (2011) 3444.
 16. Pivac N, Diksic M. The lumped constant of α -methyl-L-tryptophan is not influenced by drugs acting through serotonergic system. *Neurochemistry Int* **58** (2011) 826.
 17. Pivac N, Nikolac M, Nedić G, Mustapić M, Borovečki F, Hajnšek S, Presečki P, Pavlović M, Mimica N, Muck-Šeler D. Brain derived neurotrophic factor Val66Met polymorphism and psychotic symptoms in Alzheimer's disease. *Progr Neuro-Psychopharmacol Biol Psychiatry* **35** (2011c) 356.
 18. Lo Muzio L, Pastorino L, Levanat S, Musani V, Situm M, Bianchi Scarra G (2011) Clinical utility gene card for: Gorlin syndrome. *Eur J Human Genet* **19** (2011) doi:10.1038/ejhg.2011.9

Review Articles

1. Grdiša M. The delivery of biologically active (therapeutic) peptides and proteins into cells. *Curr Med Chem* **18** (2011) 1373.
2. Slade N, Horvat A. Targeting p73 - a potential approach in cancer treatment. *Curr Pharmaceut Design* **17** (2011) 591.
3. Borovecki F, Natasa Klepac, Dorotea Muck-Seler, Sanja Hajnsek, Zdenko Mubrin, Pivac N (2011) Unraveling the biological mechanisms in Alzheimer's disease – lessons from genomics. *Progr Neuro-Psychopharmacol Biol Psychiatry* **35** (2011) 340
4. Gotovac K, Pivac N, Hajnšek S, Muck-Šeler D, Borovečki F. Quest for New Genomic and Proteomic Biomarkers in Neurology. *Transl Neurosci* **2** (2011) 69.
5. Muck-Šeler D, Pivac N. Serotonin: an overview. *Period Biol* **113** (2011) 29.

BOOK CHAPTERS:

1. Pivac N, Nedić G, Nikolac M, Mustapić M, Švob Štrac D, Jazvinščak Jembrek M, Mück-Šeler D. Molecular mechanisms of traumatic brain injury. In: Traumatic brain injury. Wounds of war III. Wiederhold Brenda K (ed). Amsterdam: IOS Press, 2011, pp 81-111.
2. Marčinko D, Pivac N, Šagud M, Muck-Šeler D, Mihaljević-Peleš A, Jakovljević M. Biological basis of suicidal behaviour (in Croatian). In: Suicidology. Marčinko D et al., Marcinko D (ed), Medicinska naklada Zagreb, 2011, pp 62-81.



DIVISIONAL ORGANIZATION

Head: Tarzan Legović

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

- ⇒ Laboratory for Aquaculture and Pathology of Aquatic Organisms, Emin Teskeredžić
- ⇒ Laboratory for Analytical Chemistry and Biogeochemistry of Organic Compounds, Marijan Ahel
- ⇒ Laboratory for Inorganic Environmental Geochemistry, Goran Kniewald
- ⇒ Laboratory for Bioelectrochemistry and Surface Imaging, Vesna Svetličić
- ⇒ Laboratory for Biological Effects of Metals, Marijana Erk
- ⇒ Laboratory for Physical Chemistry of Traces, Milivoj Lovrić
- ⇒ Laboratory for Physical Chemistry of Aquatic Systems, Irena Ciglonečki Jušić
- ⇒ Laboratory for Geochemistry of Colloids, Ivan Sondi
- ⇒ Laboratory for Informatics and Environmental Modelling, Tarzan Legović
- ⇒ Laboratory for Molecular Ecotoxicology, Tvrtko Smital
- ⇒ Laboratory for Radioecology, Delko Barišić
- ⇒ Satellite Oceanography Laboratory, Milivoj Kuzmić



OVERVIEW OF THE DIVISION

Division contributions include fundamental and applied research in marine, freshwater and terrestrial systems, processes and states. This research is oriented toward the optimization of environmental management for the benefit of our country and the world. During 2011, division scientists worked on more than 50 research projects contracted by the Ministry of Science, Education and Sport and outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from satellite oceanography to nanotechnology. Research results were published in 63 scientific papers in journals indexed by Current Contents, 2 book chapters and a number of conference proceedings. In addition, division scientists gave 18 invited lectures, organized 8 conferences and acted as coordinators for 4 graduate schools. 4 Ph.D, 3 M.Sc and 3 B.Sc. theses were completed under the mentorship of division scientists. Finally, 7 undergraduate and 50 post-graduate courses were given at universities in Croatia and abroad.



Fig. 1. Research station Martinska, summer 2011.

TOP ACHIEVEMENTS

Identification of novel biotransformation products of macrolide and fluoroquinolone antimicrobials

Several novel biotransformation products (TPs) of macrolide and fluoroquinolone antimicrobials were identified in wastewater effluents from a membrane biological reactor (MBR) using ultrahigh-performance liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (UPLC-QToF). A semi-quantitative assessment of these TPs suggested that they might have contributed significantly to the overall balance of antimicrobial residues in MBR effluents (Terzić et al., 2011).

Functioning of a PCB-degrading bacterial community in long-term contaminated soil under bioremediation

A small-scale bioremediation assay was developed in order to gain insight into the functioning of a polychlorinated biphenyl (PCB) degrading community during the bioremediation of contaminated soil. Two bioremediation strategies, including biostimulation and bioaugmentation with selected seed cultures, were applied in order to en-

hance the removal of PCBs from contaminated soil. Faster PCB reduction was achieved in bioaugmented soils suggested an important role for seed cultures in bioremediation processes (Petrić et al., 2011).

Cellular energy allocation in mussels as a physiological biomarker

This study demonstrates the usefulness of cellular energy allocation (CEA) evaluations as a physiological biomarker to infer the occurrence of natural stress in native populations of mussels inhabiting the stratified estuary (Krka River estuary, Croatia). Decreases in CEA recorded in estuarine mussels may ultimately result in a lower amount of energy available for growth, reproduction, or defence against other stressors (e.g. pollution) (Erk et al., 2011).

Rogoznica Lake, an ideal study site for bio-geochemical processes in euxinic environments

A new model for molybdenum behavior in euxinic basins was developed based on Mo behaviour in the sulfidic anoxic water column of Rogoznica Lake. The existence of a new Fe-Mo-S mineral is postulated; its composition is inferred to approximate $\text{FeMo}_0.6\text{S}_{2.8}$ and its solubility was determined. It was shown that the detected sulfur species highly influenced the electrochemical measurement of copper and copper complexing capacity determination, through contributions to copper ion binding. The observed high sulfur isotope fractionation between sulfate and sulfide in the lake is likely to result from bacterial sulfate reduction, unaccompanied by bacterial sulfur disproportionation (Helz et al. 2011).

Application of Brewster angle microscopy and fractal analysis in investigations of compressibility of

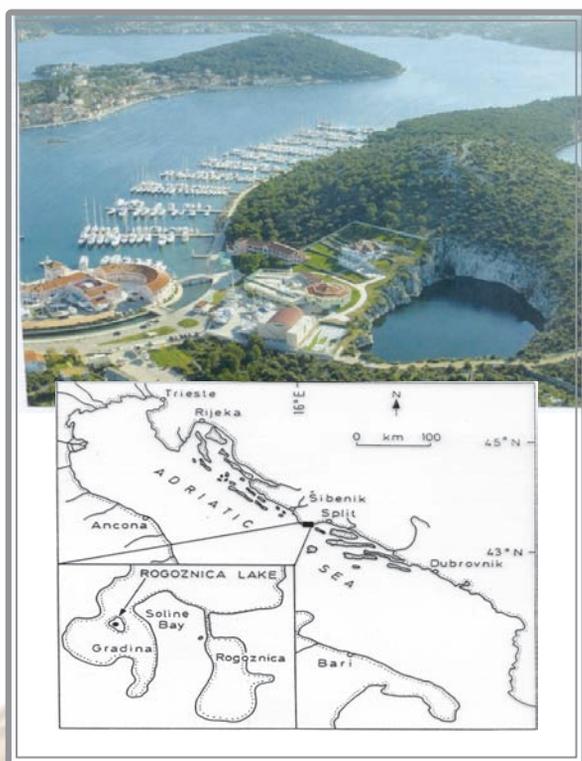


Fig. 2. Rogoznica lake, Eastern Adriatic coast, Croatia.

Langmuir monolayers

The connection between the lipid/amphiphile monolayer structure at the interface and its macroscopic/rheological properties was investigated by using fractal analysis of images obtained by Brewster angle microscopy (BAM) to infer the fractal dimension of the monolayer structure and relate its change to the corresponding changes in compressibility derived from p-A isotherm. The results provide unambiguous identification of onset of percolation in a Langmuir layer and should facilitate a more efficient application of percolation theory in the study of processes and structures at the interface during monolayer compression (Risović et al., 2011).

Organic matter study in the Northern Adriatic as a key for its functioning

A study of organic matter in the northern Adriatic, including surface-active organic

substances and lipid classes, in combination with measurements of nutrients, chlorophyll a and phytoplankton composition and abundance, revealed that the major influential parameters for organic matter production and remineralization are nutrient status, dominant phytoplankton fraction and bacterial activity. We recently observed that increasing oligotrophy leads to increased biosynthesis of lipids, mainly glycolipids, and to an increased number of phytoplankton taxa (Frka et al., 2011).

Assessment of copper, cadmium and zinc remobilization in Mediterranean marine coastal sediments

The remobilization of copper, cadmium and zinc in the sediments of three selected coastal microenvironments of the Aegean Sea (Eastern Mediterranean) was assessed. Various analytical methods and techniques were employed to measure concentrations, profiles and forms of metals and organic matter in sediments and pore waters, which is of great significance for their fate in the marine environment and their toxicity (Sakellari et al., 2011).

Anthropogenic impacts on the pristine area of the Plitvice lakes

Analysis of dated sediment cores from the pristine area of the Plitvice lakes indicated recent input of typical anthropogenic contaminants such as P and PAH. They originate from fossil fuels and anionic surfactants which indicate leakage of untreated wastewater into the lakes. An interesting natural geological anomaly leading to high Cd levels in all sediments was observed (Mikac et al., 2011).

Anthropogenic and natural influences on the mineral content of wines from Croatia

Wines from several regions of Croatia (Slavonia, Istria) and Vojvodina were analysed for the content of 25 elements. Regional differences based on geogenic elements were observed. Cd, Ni, Zn, Fe and Cr were found to be primarily of anthropogenic origin and a geochemical arsenic anomaly in Slavonia contributed to higher As values in wines from this region (Fiket et al., 2011).

Development of a novel method for identification of the type and potency of fish P-glycoprotein (abcb1) substrates and inhibitors

P-glycoprotein (P-gp; abcb1) is one of the major ABC transport proteins that mediates multixenobiotic resistance (MXR) defense in fish. In order to offer a sound evaluation of its ecotoxicological relevance, a specific ATPase assay for identification of fish P-gp environmental substrates and inhibitors was developed using P-gp enriched membrane vesicles isolated from fish hepatoma PLHC-1/dox cells characterized by high overexpression of P-gp (Žaja et al., 2011).

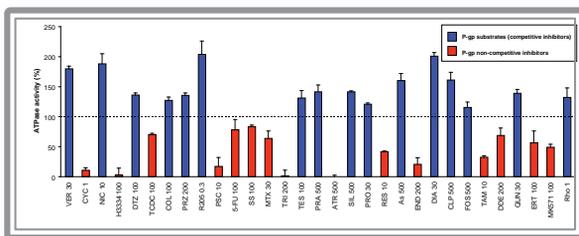


Fig. 3. Identification of fish P-gp substrates and inhibitors using the ATPase assay. Baseline ATPase activity is set at 100%. Compounds that show activity higher than 100% are identified as P-gp substrates (potential competitive inhibitors), while the ones with activity lower than 100% are identified as non-competitive P-gp inhibitors.

Metal pollution in sediments from the Rijeka harbour

Metal pollution in sediments from the Rijeka harbour were found to be comparable with other world port sediments. Based on 63 measured elements, Hg was found to be the most prominent pollutant with concentrations

exceeding 4 mg/kg. Metal pollution was found to be decreasing during the last decades, except for Ag and Ba contamination (Cukrov et al., 2011).



Fig. 4. Water sampling at the river Sutla for basic physico-chemical parameters.

Polymer Networks produced by Marine Diatoms in the Northern Adriatic Sea

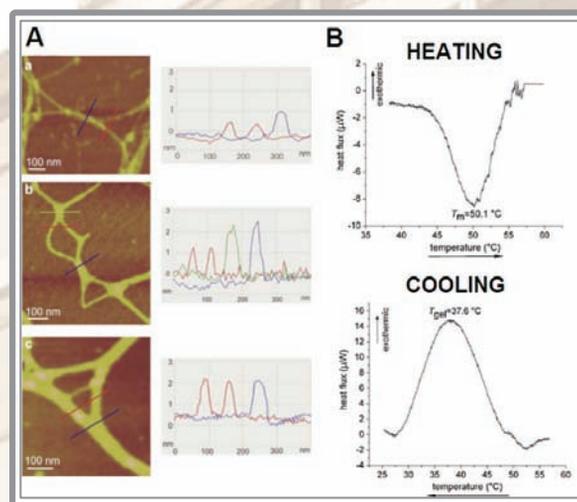


Fig. 5. Structural details of the gel network at molecular resolution. The fibril associations are presented as topographical AFM images with characteristic vertical profiles of fibrils forming junction zones (A). Heating and cooling DSC thermographs of marine gel (B)

Using a high resolution molecular AFM technique, we addressed the extracellular polymer production of the Adriatic diatom *Cylindrotheca closterium*. Analyses were performed at the single cell level and at the level of supramolecular organization of a gel phase isolated from Northern Adriatic macroaggregates. Our results revealed that extracellular polysaccharides freshly produced by marine diatoms can self-assemble directly to form a gel network characteristic of the macroscopic gel phase in the natural aquatorium, independent on any bacterial mediation or interaction with inorganic particles (Svetličić et al., 2011).

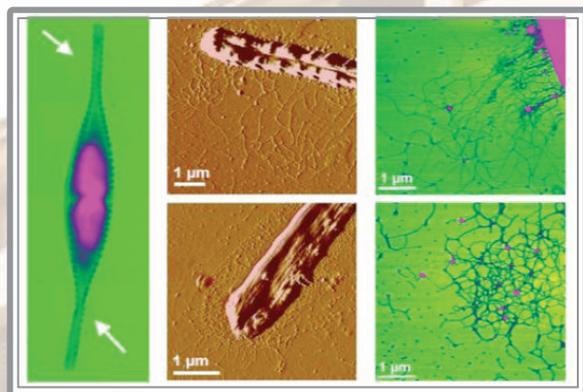


Fig. 6. Extracellular polymeric substance release by marine diatom *Cylindrotheca closterium* imaged by atomic force microscopy

Finfish Mariculture Dynamic Energy Budget Model

Kinetics of the isothermal crystallization of teA new theoretical framework is proposed for devising feeding strategies in aquaculture, and a complete lifecycle model aimed at understanding metabolism of one of the most lucrative aquaculture species – pacific bluefin tuna (PBT). Application of the new tools to sea bream aquaculture suggested significant improvements if feeding for smaller fish was increased. High maintenance requirements, most likely fueled by high energy expenditure on movement – were identified as the main reason for extremely inefficient

aquaculture production of PBT (Jusup et al., 2011).

NEW EQUIPMENT

1. New Ultra Low Level Liquid Scintillation Counter
2. High quality Langmuir-Blodgett trough with reflection spectrometer
3. Anoxic glove box
4. PGSTAT 128N Electrochemical analyser with EQCM module and automatic VA Stand 663 Hg electrode

EDUCATION

Division members teach at all universities in Croatia and some universities abroad. In addition, they help coordinate four Ph.D. schools: *Environmental Management and Oceanology* with the University of Zagreb, *Biophysics* with the University of Split, and *Environmental Protection and Nature Conservation* with the University J.J. Strossmayer in Osijek.

AWARDS

1. Galja Pletikapić, Bruker award for technically and visually outstanding AFM image (2011)
2. Irena Ciglencečki-Jušić; Tarzan Legović, Members, Scientific Council on Marine Science, Croatian Academy of Science and Art, Zagreb, Croatia

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Interactions of trace metal species in an aquatic environment. Program leader: Ivanka Pižeta
2. Biogeochemistry of metals in sedimentary

- systems and soils in Croatia. Program leader: Goran Kniewald
3. Nature of organic matter, interaction with traces and surfaces in environment. Program leader: Zlatica Kozarac
 4. Metal-induced cellular changes in aquatic organisms. Program leader: Biserka Raspor
 5. Organic compounds as molecular markers of anthropogenic impact on the environment. Program leader: Marijan Ahel
 6. Nanoparticles in biogeochemical processes in the environment. Program leader: Ivan Sondi
 7. Surface force on atomic scale applied in marine science and nanotechnology. Program leader: Vesna Svetličić
 8. Mathematical modeling of circulation and satellite sensing of boundary processes. Program leader: Milivoj Kuzmić
 9. Pathology of aquatic organisms in relation to pollution and aquaculture. Program leader: Emin Teskeredžić
 10. Ecological modelling for sustainable management of resources. Program leader: Tarzan Legović
 11. Radionuclides and trace elements in environmental systems. Program leader: Delko Barišić
 12. Electroactive films for ecologically acceptable conversion and energy storage. Program leader: Višnja Horvat-Radošević
 13. Electroanalytical research of microcrystal and traces in dissolved substances. Program leader: Milivoj Lovrić
 14. Information systems for environmental quality and risk assessment. Program leader: Jadranka Pečar-Ilić
 15. Ecotoxicological significance of ABC transport proteins in aquatic organisms. Program leader: Tvrtko Smital
 16. Networked Economy. Program leader: Jadranka Pečar-Ilić
 17. Systematic study of the Adriatic Sea as a basis for sustainable development of the Republic Croatia, Croatian National Monitoring Programme of the Adriatic Sea.

Research, developmental and international projects

1. Development of nanotechnology-based sensor for bio-molecules (Croatian Science Foundation), Vesna Svetličić
2. Reference Laboratory for water testing laboratories in Croatia, Ministry of Regional Development, Forestry and Water Management, Water Management Directorate), Biserka Raspor; Zlatica Kozarac; Dubravka Hršak; Božena Čosović
3. Adhesion of liposomes at electrode, Croatia-Slovenia cooperation in science and technology, Nadica Ivošević DeNardis
4. Supramolecular organization of polysaccharide network in marine gels, Croatia-Slovenia cooperation in science and technology, Vesna Svetličić
5. Investigation of the pollution of Croatian and Slovenian Northern Adriatic coast by organotin compounds and toxic metals with different analytical techniques, Slovenian-Croatian project, Nevenka Mikac
6. Integration of geo-chemical laboratory techniques, in situ field measurement, and hyperspectral air-borne remote sensing for environmental risk assessment, Hungarian-Croatian bilateral cooperation, Stanislav Frančičković-Bilinski
7. On line toxicity sensors based on modification of membrane organisation, NATO science for peace and security programme, Blaženka Gašparović; L.A. Nelson
8. Metal exposure and associated effects in mussels: An integrated approach – hyphenated analytical techniques and biomarkers, Croatian-German bilateral collaboration (DAAD), Marijana Erk; Andreas Prange
9. Complex investigation of organic aerosols in rural, urban and marine environment, Bilateral collaboration with Hungary, Zlatica Kozarac; G. Kiss
10. Determination and behaviour of organotin compounds on the Eastern Adriatic, French-Croatian bilateral project COGITO, Nevenka Mikac
11. Influence of HE Miljacka on ecosystem of

- lake Brljan“, NP Krka, Irena Ciglencečki-Jušić
12. Biogeochemistry of sulfur, carbon, nutrients and redox sensitive elements in hypoxic/anoxic aquatic environments. Bilateral collaboration with State Key Laboratory of Marine Environmental Science, Xiamen University, China, Irena Ciglencečki-Jušić; Minhan Dai
 13. Development and evaluation of innovative tools to estimate the ecotoxicological impact of low dose pesticide application in agriculture on soil functional microbial biodiversity. ECOFUN-MICROBIODIV (under SEE-ERA.NET PLUS Joint Call), Ines Petrić
 14. Radiochemical methods for determination of radionuclides in water samples“, Croatian – Slovenian bilateral cooperation, Martina Rožmarić Mačefat
 15. Nanoparticles in aqueous environment: electrochemical, nanogravimetric, STM and AFM studies, UKF project, Irena Ciglencečki-Jušić; Nikola Batina
 16. Hidrogeological studies of the Kupa River and its tributaries“, Croatian – Austrian bilateral cooperation, Stanislav Frančišković-Bilinski
 17. European network on applications of atomic force microscopy to nanomedicine and life science. COST Action (2010-2014). WG 4: Environmental Nanotoxicology and Nanoparticles, Coordinator Vesna Svetličić . National representatives: Vesna Svetličić; Amela Hozić
 18. Radiological monitoring in Croatia, Nuclear Power Plant Krško, Željko Grahek
 19. Determination of radioactivity in the Danube River in 2011., Delko Barišić
 20. The program of systematic testing and monitoring of radioactive substances in the sea – sessile indicator organisms (National Institute of Radiological and Nuclear Safety), Delko Barišić
 21. Measurement of radioactivity in liquid effluents of Nuclear Power Plant Krško, Željko Grahek
 22. Monitoring of freshwater fishery: fishing area of the Rivers Kupa, Korana, Dobra and Mrežnica“, Ministry of Agriculture, Fishery and Rural Development, Emin Teskeredžić
 23. Anthropogenic influence (ecotoxic metals) research in the sediments of Brljan Lake and downstream lakes, Neven Cukrov
 24. Trace metals analysis in subterranean waters of Petruševac water well's, Cukrov, Neven
 25. Determination of ecotoxic metals in water environment of Rijeka harbor using passive samplers, (2011-2012), Neven Cukrov
 26. Environmental impact assessment of the upcoming beach Crnica, (2011), Neven Cukrov
 27. Analysis of heavy metals concentrations (Hg, Cd, Pb, Cu & Zn) in the sediments of Šibenik port, (2011), Neven Cukrov
 28. Significado ambiental (climático e hidrológico) de registros tobáceos fluviales de la Cordillera Ibérica monitorizados entre 1999 y 2009. Comparación con otros registros recientes y antiguos. Project Spanish Ministry of Science and Innovation, (2010-2012), Neven Cukrov
 29. Finfish Mariculture Dynamic Energy Budget Model - FiMDEB“, Unity Through Knowledge Fund, Tin Klanjšček
 30. The ocean chemistry on bioactive trace elements and paleoclimate proxies', COST action, Irena Ciglencečki-Jušić
 31. On determination natural metal concentrations in waters according to Water Framework Directive, Croatian Waters, Marina Mlakar
 32. Determination of ecotoxic trace metals in water, sediments and biota of Nature Park „Telaščica“ aquatorium, Ministry of environmental and nature protection, Marina Mlakar
 33. Influence of the water mass circulation on spatial and temporal distribution of ecotoxicants in Malo jezero and Veliko jezero lakes of Mljet National Park, Vlado Cuculić
 34. An impact of antifouling paints as a source of contamination by ecotoxic metals in the coastal marine environment, French-Croatian COGITO project, Dario Omanović; Cedric Garnier
 35. Gold microwire: a new tool for trace metal speciation in natural waters, The Royal Society project, Pascal Salaun; Dario Omanović
 36. Water quality in the Bay of Pag, Agrokor, Marta Plavšić

INVITED LECTURES

1. Ahel M, Comprehensive Scheme for Non-target Screening of Wastewater and Its Application for the Effect-directed Analysis Municipal Sewage, 13th EuCheMS International Conference on Chemistry and the Environment (ICCE 2011), Zurich, September 11-15, 2011
2. Ahel M, Effects-directed Analysis of Contaminated Sediments from the Sava River, Croatia // SETAC Europe Annual Meeting: Ecosystem Protection in a Sustainable World: A Challenge for Science and Regulation. Milano, Italy, May 15-19, 2011
3. Ciglencečki-Jušić I. Rogoznica Lake (Dragon Eye) – a unique aquatic system on the Adriatic coast, RBI, Zagreb, Croatia, June 9th, 2011.
4. Ciglencečki-Jušić I. Brief Overview on Rogoznica Lake field work. Xiamen University, Xiamen China, October 27th, 2011.
5. Dutour Sikirić M, Perfect forms and perfect Delaunay. Ben Gurion University of the Negev, BGU Seminar on Algebraic Combinatorics, Beer Sheva Israel, November 24, 2011
6. Erk M, Metals as contaminants and their effects on aquatic organisms. Bilateral Croatian-German project (DAAD), Helmholtz-Zentrum Geesthacht, Institute of Coastal Research/Operational Systems, Department of Marine Bioanalytical Chemistry, Geesthacht, Germany, June 20, 2011
7. Frka S, "To develop tools for assessing global air-sea fluxes of climate and air pollution relevant gases", workshop related to Cost Actions 735, Plymouth, UK. January, 25-26, 2011.
8. Gašparović B, What is the sea surface microlayer? Towards an unified physical, chemical and biological definition of the air-ocean interface", workshop related to the COST Action 735 programme (www.cost-735.org), Plymouth, UK, January 25-26, 2011
9. Jusup M, Klanjšček T, Matsuda H, Kooijman S.A.L.M, A full lifecycle bioenergetic model for bluefin tuna. DEB Symposium 2011, Lisbon, Portugal, April 13-15, 2011
10. Kniewald G, Environmental issues related to the use of depleted uranium ordnance during the Kosovo conflict. IX International Conference on Military Geosciences, Las Vegas, USA, June 20-24, 2011
11. Legović T, The biggest disaster performed by humanity in the second part of the 20th century: world's fishery and the role of modelers. 7th European Conference on Ecological Modelling, Riva del Garda, Italy, May 30 – June 02, 2011
12. Legović T, Effect of maximum sustainable yield on marine ecosystems. Institute of Oceanography and Fisheries, Split, Croatia, November 24, 2011
13. Legović T, Marine pollution with cigarette butts. Croatian Television, Zagreb, August 11, 2011
14. Marguš M, "Nanoparticles in natural environment: electrochemical and AFM, STM studies" Xiamen University, Xiamen China
15. Milanović I, "Nanoparticles in natural environment: electrochemical and DLS studies" Xiamen University, Xiamen China
16. Omanović D, "Element speciation in the Toka river (Hungary) impacted by an abandoned mine effluents assessed by DGT technique", Université du Sud Toulon Var, La Garde, France, September 29, 2011.
17. Pižeta I, An adaptable Automatic Trace metal Monitoring System for on line measuring in natural waters, Université du Sud Toulon Var, La Garde, France, October 04, 2011
18. Pižeta I, The role of statistics in the interpretation of measurement results from the environment, Université du Sud Toulon Var, La Garde, France, October 20, 2011

ORGANIZED CONFERENCES

1. Satellite Student Regional Symposium on Electrochemistry. Rudjer Boskovic Institute, March 3, 2011. Organizer: Jadreško, Dijana
2. Croatian fishery at the entrance of EU: Fish as a functional food. Vukovar, Croatia, April 7-9, 2011. Members of organizing committee: Teskeredžić, Zlatica; Teskeredžić, Emin
3. Thirty years of research at the station Martinska. Šibenik, May 11, 2011. Organizers: Mihelčić, Goran; Legović, Tarzan

4. Meeting of the NATO Final project SFP 983147, Dubrovnik, Croatia, May, 17-18, 2011
5. Conference on monitoring lake water and sedimen (project SOWAEUMED), Plitvice lakes, Croatia, May 29 - June 1, 2011
6. Symposium of RBI young reseachers "Scientific meeting of the 3rd kind", Ruđer Bošković Institute, July 7-8, 2011. Member of the Organizing Committee: Filipović Marijić, Vlatka; Vardić Smrzlić, Irena; Valić, Damir, Čadež, Vida; Penezić, Abra, Klanjšček, Tin.
7. IVth International Meeting on AFM in Life Sciences and Medicine, Paris, France, August 23-27, 2011. Member of organizing committee: Svetličić, Vesna; Member of the local organizing committee Hozić, Amela
8. 9th International Microsymposium on Electrochemical Impedance Analysis, June, 02-05. 2011, Sv. Andrija/Rovinj, Croatia. Members of Local Organizing Committee: Horvat-Radošević, Višnja; Magdić, Katja
7. Frka S, Gašparović B, Marić D, Godrijan J, Đakovac T, Vojvodić V, Dautović J, Kozarac Z. Phytoplankton driven distribution of dissolved and particulate lipids in the northern Adriatic (Mediterranean) : Spring to summer situation. *Estuar Coast Shelf Sci* **93** (2011) 290.
8. Furdek M, Vahčić M, Ščančar J, Milačić R, Kniewald G, Mikac N. Organotin compounds in seawater and mussels *Mytilus galloprovincialis* along the Croatian Adriatic coast. *Mar Pollut Bull* **64** (2012) 189.
9. Helz G.R, Bura-Nakić E, Mikac N, Ciglencečki I. New model for molybdenum behavior in euxinic waters. *Chem Geol* **284** (2011) 323.
10. Jusup M, Klanjšček T, Matsuda H, Kooijman, S.A.L.M. 2011. A Full Lifecycle Bioenergetic Model for Bluefin Tuna. *PLoS ONE* **6** (2011) e21903.
11. Kosanović C, Havenscak K, Subotić B, Svetličić V, Mišić Radić T, Cziraki A, Huhn G, Buljan I, Smrečki V. Study of the mechanism of formation of nano-crystalline zeolite X in heterogeneous system. *Micropor Mesopor Mat* **142** (2011) 139.
12. Mikac I, Fiket Ž, Terzić S, Barešić J, Mikac N, Ahel M. Chemical indicators of anthropogenic impacts in sediments of the pristine karst lakes, *Chemosphere* **84** (2011) 1140..
13. Molnár P.K, Derocher A.E, Klanjšček T, Lewis M.A.. Predicting climate change impacts on polar bear litter size. *Nat Commun* **2/186** (2011).
14. Muller E.B, Ananthasubramaniam B, Klanjšček T, Nisbet R.M. Entrainment of cell division in phytoplankton with dynamic energy budgets. *J Sea Res* **66** (2011) 447.
15. Petrić I, Bru D, Udiković-Kolić N, Hršak D, Philippot L, Martin-Laurent F. Evidence for shifts in the structure and abundance of the microbial community in a long-term PCB-contaminated soil under bioremediation. *J Hazard Mat* **195** (2011) 254.
16. Risović D, Frka S, Kozarac Z. Application of Brewster angle microscopy and fractal analysis in investigations of compressibility of Langmuir monolayers. *J Chem Phys* **134** (2011) 024701-1-024701-9.

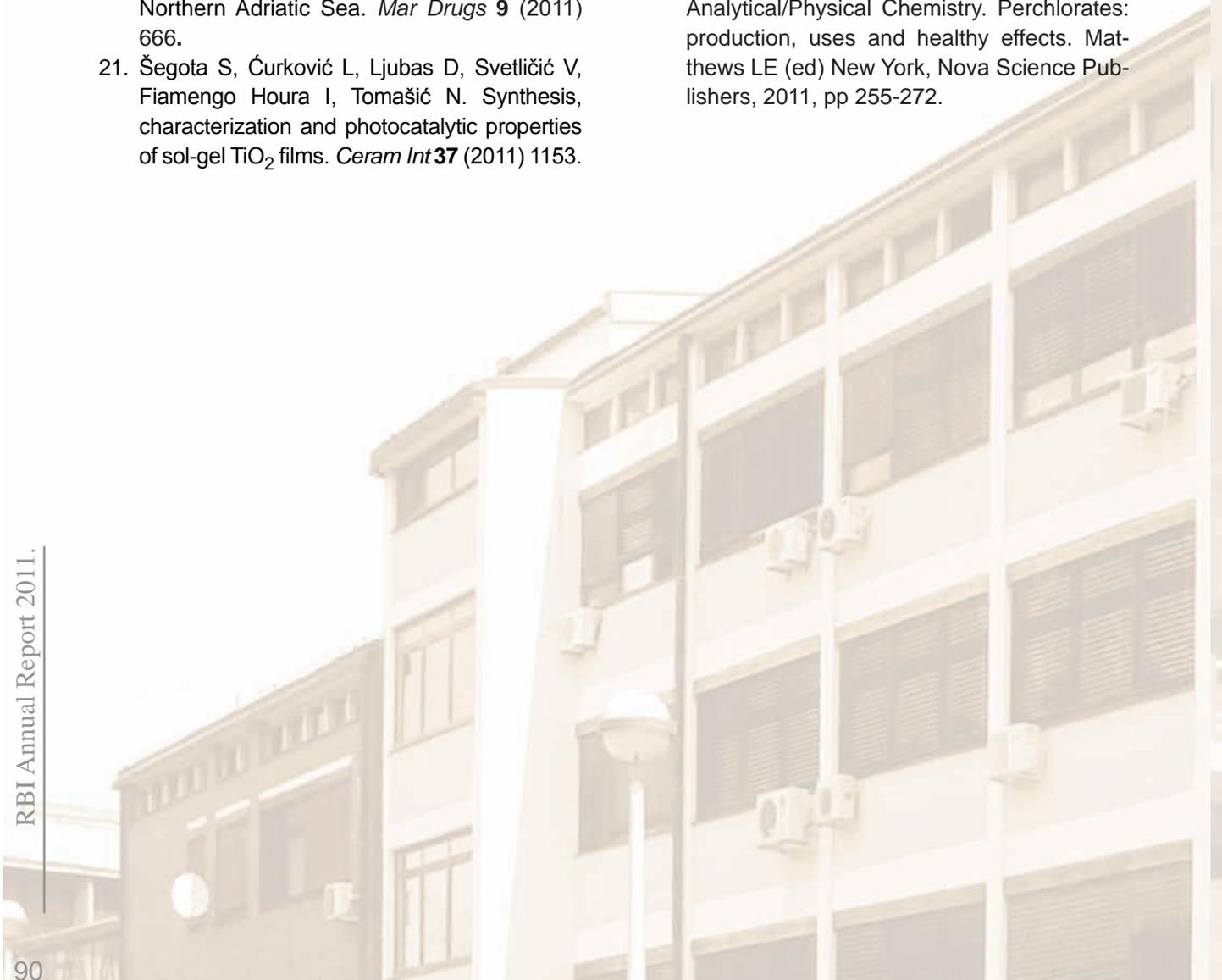
SELECTED PUBLICATIONS

1. Biljan I, Kralj M, Mišić Radić T, Svetličić V, Vančik H. Dimerization of Nitrosobenzene Derivatives on an Au(111) Surface. *J Phys Chem C* **115** (2011) 20267.
2. Bura-Nakić E, Krznarić Dr; Helz G.R, Ciglencečki-Jušić I. Characterization of Iron Sulfide Species in Model Solutions by Cyclic Voltammetry. Revisiting an Old Problem. *Electroanalysis* **23** (2011) 1376.
3. Cuculić V, Cukrov N, Kwokal Ž, Mlakar M. Distribution of trace metals in anchialine caves of Adriatic Sea, Croatia. *Estua Coast Shelf Sci* **95** (2011) 253.
4. Cukrov N, Frančišković-Bilinski S, Barišić D, Hlača B. A recent history of metal accumulation in the sediments of Rijeka harbour, Adriatic Sea, Croatia. *Mar Pollut Bull* **62** (2011) 154.
5. Erk M, Ivanković D, Strižak Ž. Cellular energy allocation in mussels (*Mytilus galloprovincialis*) from the stratified estuary as a physiological biomarker. *Mar Pollut Bull* **62** (2011) 1124.
6. Fiket Ž, Mikac N, Kniewald G. Arsenic and other trace elements in wines of eastern Croatia, *Food Chem* **126** (2011) 941.

17. Sakellari A, Plavšić M, Karavoltsos S, Dasenakis M, Scoullou M. Assessment of copper, cadmium and zinc remobilization in Mediterranean marine coastal sediments. *Estuar Coast Shelf Sci* **91** (2011) 1.
18. Slade D, Dunstan M.S, Barkauskaite E, Weston R, Lafite P, Dixon N, Ahel M, Leys D, Ahel I. The structure and catalytic mechanism of a poly(ADP-ribose) glycohydrolase. *Nature* **477** (2011) 616.
19. Superville P.J, Louis Y, Billon G, Prygiel J, Omanović D, Pižeta I. An adaptable automatic trace metal monitoring system for on line measuring in natural waters. *Talanta* **87** (2011) 85.
20. Svetličić V, Žutić V, Mišić Radić T, Pletikapić G, Hozić Zimmermann A, Urbani R. Polymer Networks produced by Marine Diatoms in the Northern Adriatic Sea. *Mar Drugs* **9** (2011) 666.
21. Šegota S, Ćurković L, Ljubas D, Svetličić V, Fiamengo Houra I, Tomašić N. Synthesis, characterization and photocatalytic properties of sol-gel TiO₂ films. *Ceram Int* **37** (2011) 1153.
22. Terzić S, Senta I, Matošić M, Ahel M. Identification of biotransformation products of macrolide and fluoroquinolone antimicrobials in membrane bioreactor treatment by ultrahigh-performance liquid chromatography/quadrupole time-of-flight mass spectrometry. *Anal Bioanal Chem* **401** (2011) 353.
23. Žaja R, Lončar J, Popović M, Smital T. First characterisation of fish P-glycoprotein (abcb1) substrate specificity using determinations of its ATPase activity and calcein-AM assay with PLHC-1/dox cell line. *Aquat Toxicol* **103** (2011) 53.

BOOK CHAPTER

1. Zelić M. Perchlorates in the Laboratory for Analytical/Physical Chemistry. Perchlorates: production, uses and healthy effects. Matthews LE (ed) New York, Nova Science Publishers, 2011, pp 255-272.



DIVISIONAL ORGANISATION

Head: Nenad Smodlaka

The Centre for Marine Research consists of the following laboratories:

- ⇒ Laboratory for marine molecular toxicology, Renato Batel
- ⇒ Laboratory for marine ecotoxicology, Nevenka Bihari
- ⇒ Laboratory for biomineralization nanostructure and radioecology, Davorin Medaković
- ⇒ Laboratory for marine microbial ecology, Mirjana Najdek
- ⇒ Laboratory for processes in the marine ecosystem, Robert Precali
- ⇒ Laboratory for ecology and systematics of benthos, Ana Travizi



TOP ACHIEVEMENTS

Acetylcholinesterase (AChE) activity in the gills of mussel (*Mytilus galloprovincialis*) from the north-eastern Adriatic coast

A significantly lower enzyme activity in comparison to the reference site was recorded at sites in close vicinity to urban and industrial areas. In addition, AChE activity decreased at a site within the area of the Limski channel. AChE reduction in the gills of mussels, recorded mostly in polluted harbours, could be related to the presence of common environmental pollutants (Perić and Petrović, 2011).

The shells of *Mytilus galloprovincialis* as a bioindicator of environmental conditions

Oxygen $\delta^{18}\text{O}$ and carbon $\delta^{13}\text{C}$ isotopes were analysed for calcite and aragonite in separate shell layers. According to the observed enrichment of $\delta^{13}\text{C}$ in aragonite and of $\delta^{18}\text{O}$ in the calcite layer the investigated area could be divided into locations with a greater influence of freshwater, those with lesser influence of freshwater and those with marine environments (Kanduč et al., 2011).

OVERVIEW OF THE DIVISION

The mission of the Center for Marine Research is the multidisciplinary study of processes in the marine environment from subcellular to regional scale, especially in plankton and benthic communities of the northern Adriatic Sea. In addition to basic research, the Center is involved in monitoring the Adriatic Sea for government purposes and several international projects relating to protection of the marine environment.

Biom mineralization and proteins in mollusc shells

The biomineralization process in mollusc shells is controlled by an array of proteins, glycoproteins and polysaccharides that collectively constitute the shell matrix. The shell matrix of the model organism *Helix aspersa maxima* snail differ widely from the shell secretory repertoire of the marine gastropod *Haliotis* or the pearl oyster *Pinctada* (Pavat et al., 2011).

Microbial communities in northern Adriatic mucilaginous aggregates: insight into the early phase of aggregate formation

The presence and activity of heterotrophic bacteria belonging to the Alteromonadaceae, regularly observed in fresh aggregates, suggest that the early phase of aggregate formation corresponds to an abrupt change of environmental conditions due to the mixing of central and northern Adriatic waters (Blažina et al., 2011).

Intrusion of high-salinity water causes accumulation of transparent exopolymer particles (TEP) in the northern Adriatic Sea

During the period of maximal TEP accumulation, a pronounced increase in the abundance of diatoms and bacteria coincided with low cell-specific production of bacterial biomass, and a low abundance of actively respiring bacteria. In contrast, during the period of lower TEP concentration an increase in the abundance of active bacteria and cell-specific β -glucosidase activity indicates enhanced degradation of TEP (Najdek et al., 2011).

Picoplankton composition related to mesoscale circulation on the Albanian boundary zone (southern Adriatic)

Picoplankton distribution was greatly influenced by hydrographic conditions prevailing in the southern Adriatic due to the influence of the Levantine Intermediate Water (LIW) and East Adriatic Current (EAC) force. LIW intrusion was followed by *Prochlorococcus* and *Synechococcus* (two ecotypes). The largest number of picoeukaryotes was observed at offshore stations, strongly influenced by EAC, which at the same time acted as a barrier for *Prochlorococcus* (Šilović et al., 2011). A distinct plankton distribution was observed on each side of the shelf break hydrographic boundary. Low nutrient concentrations influence the relatively low productivity not only above the Albanian shelf but also further to the north along the Montenegrin and Croatian coastal Adriatic Sea (Viličić et al., 2011).

Impact of circulation on high phytoplankton blooms and fish catch in the northern Adriatic (1990-2004)

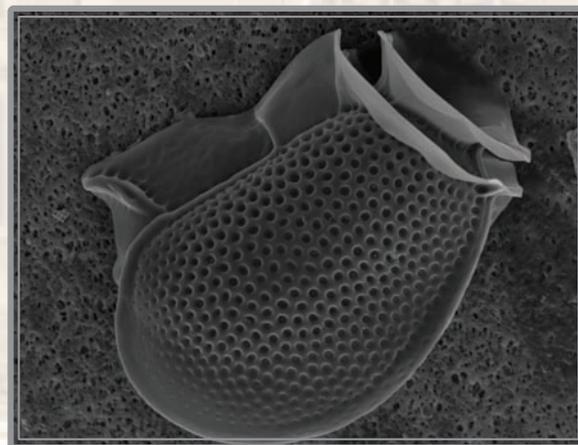


Fig. 1. *Dinophysis fortii*, phytoplankton species.

The intensity and duration of northern Adriatic phytoplankton blooms was highly related to specific oceanographic conditions. Blooms appeared in separate circulation cells with different species distribution. The hypothesis that specific northern Adriatic oceanographic conditions in February play

a key role in the Adriatic anchovy stock was introduced (Kraus and Supić, 2011).

Similar content of SAS at two eutrophic different stations in the northern Adriatic

Despite notably different nutrient and Chl concentrations, the content of surface-active organic substances was similar at two research stations characterized by different eutrophication degrees. This effect could be ascribed to an efficient remineralization of SAS at the more eutrophic station 101, and/or different composition of the phytoplankton community between the two stations. In fact, at station 107 the nanophytoplankton fraction is more dominant, and carbon excretion rates are comparable achieving levels up to the same order of magnitude as net carbon production (Gašparović et al., 2011).

Long term changes in northern Adriatic polychaete assemblages following a dystrophic crisis

The analyses of 20 years of data on polychaete assemblages in an area that suffered a mass mortality due to dystrophic crises highlighted the importance of analysing a long-term dataset in order to understand assemblage dynamics following strong disturbance events. Our results suggested that polychaete fauna is still recovering even 20 years after the anoxic event (Mikac et al., 2011).

Spatio-temporal variability of meiofauna in isolated and unstable marine habitat

The effect of abiotic parameters on the structure and dynamics of meiofauna was studied in the shallow and isolated area of Velike Soline - an environment of high temperature and salinity fluctuations. Considering the structure of meiofauna we distinguished three zones: marine, transitional

and lagoonal, which differ with respect to the density and percentage of certain taxa, dominance pattern and habitat heterogeneity. No seasonality in meiofauna dynamics has been recorded (Cvitković et al., 2011).

Long term changes in northern Adriatic bivalve assemblages following a dystrophic crisis

Long term changes in bivalve assemblages of the muddy detritic bottom were studied comparing the data set following a dystrophic crisis in the northern Adriatic (1989-1991) with a data set characterized by an absence of dystrophic events in the period 2003-2005,. Results based on temporal changes in the functional structure and diversity of bivalves indicate that bivalve assemblages could serve as excellent indicators of disturbance and ecosystem instability (Nerlović et al., 2011).

EDUCATION

The Center is involved in the organisation of Marine Sciences Studies (undergraduate) at the Juraj Dobrila University in Pula. The majority of courses are organized by the Center's scientists. Undergraduate and postgraduate courses were given at the Universities of Zagreb, Osijek, Split, and Dubrovnik.



Fig. 2. Center for Marine Research, Rovinj

RBI Director's Award for Scientific Excellence

1. Sandi Orlić – HZZ Project -Biodiversity and biotechnological characterisation of Adriatic bacteria

PROJECTS

Programs supported by the Ministry of Science, Education and Sport

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

Projects supported by the Ministry of Science, Education and Sport

1. Impact of pollution on programmed biosynthesis in marine invertebrates, Renato Batel
2. Ecotoxic effect of contamination on marine organisms, Nevenka Bihari
3. Mathematical modelling of circulation and satellite sensing of boundary processes, Milivoj Kuzmić
4. Biomineralization processes in marine organisms, Davorin Medaković
5. Structure and physiology of microbial communities in northern Adriatic front, Mirjana Najdek
6. Mechanisms of long-term changes in the northern Adriatic ecosystem, Robert Precali
7. Biodiversity of benthic communities in the Adriatic: natural and human impacts, Ana Travizi

Research, developmental and international projects

1. The Adriatic Sea monitoring program (Coastal cities water pollution control project), Rober Precali, Ministry of Environmental protection, Construction and Physical planning, Republic of Croatia , IBRD 7226/HR
2. Molecular and physiological bacterial diversity of the trophic gradients in the Adriatic Sea, Mirjana Najdek Dragić, Ministry of Science, Education and sport, Republic of Croatia and Ministry of Science, Republic of Montenegro

3. Picoplankton function and diversity along northern Adriatic trophic gradients, Maria Blažina, Adris Foundation, Republic of Croatia
4. Biomineralization processes during embryonic development of marine organisms: gastropods, bivalves and echinoderms, Daniel M. Lyons, DAAD Germany and Ministry of Science, Education and Sport, Republic of Croatia
5. Development of nanotechnology-based sensors for bio-molecules, Daniel M. Lyons, Croatian Science Foundation, Republic of Croatia
6. Development of applied sensors for marine biotoxins, Daniel M. Lyons, Adris Foundation, Republic of Croatia
7. Seasonal changes in picoplankton composition in the Northern Adriatic Sea as assessed by CARD-FISH and Fingerprinting, Sandi Orlić, DAAD Germany and Ministry of Science, Education and Sport, Republic of Croatia
8. Biodiversity and biotechnological characterization of bacteria of the Adriatic Sea, Sandi Orlić, Croatian Science Foundation, Republic of Croatia
9. Biomineralization: Understanding of basic mechanisms for the design of novel strategies in nanobiotechnology (Biomintec), Renato Batel, EU FP7 (Marie Curie mobility)

ORGANIZATION OF CONFERENCES, CONGRESSES AND MEETINGS

1. 36th European Marine Biology Symposium, Rovinj, Croatia, 12-16.09.2011. (Organisation Committee: Ana Travizi, Maja Fafanđel, Ljiljana Iveša, Romina Kraus)
2. 2 JOINT Workshop / MC Meeting, COST Action TD0903, Understanding and manipulating enzymatic and proteomic processes in biomineralization., January 12-14, 2011, Newcastle upon Tyne, UK (Davorin Medaković)
3. 3 JOINT Workshop / MC Meeting, COST Ac-

tion TD0903, Understanding and manipulating enzymatic and proteomic processes in biomineralization., October 11-13, 2011, Cluj Napoca, Romania (Davorin Medaković)

SELECTED PUBLICATIONS

1. Kanduč T, Medaković D, Hamer B. *Mytilus galloprovincialis* as a Bioindicator of Environmental Conditions: the Case of the Eastern Coast of the Adriatic Sea. *Isot Environ Health Stud* **47** (2011) 42.
2. Gašparović B, Djakovac T, Tepić N, Degobbis D. Relationships between surface-active organic substances, chlorophyll a and nutrients in the northern Adriatic Sea. *Cont Shelf Res* **31** (2011) 1149.
3. Kraus R, Supić N. Impact of circulation on high phytoplankton blooms and fish catch in the northern Adriatic (1990-2004). *Estuar-Coast Shelf Sci* **91** (2011) 198.
4. Pavat C, Zanella-Cléon I, Becchi M, Medakovic D, Luquet G, Guichard N, Alcaraz G, Dommergues JL, Serpentine A, Lebel JM, Marin F. The shell matrix of the pulmonate land snail *Helix aspersa maxima*. *CompBiochem Physiol B-Biochem Mol Biol*. Available on line 16 December 2011 <http://dx.doi.org/10.1016/j.cbpb.2011.12.003>.
5. Mikac B, Musco L, Đakovac T, Giangrande A, Terlizzi A. Long term changes in North Adriatic soft-bottom polychaete assemblages following a dystrophic crisis. *Ital J Zoolog* **78** (2011) 304.
6. Cvitković I, Travizi A, Despalatović M, Grubelić I, Bogner D, Nikolić V, Žuljević A, Antolić B. Spatio-temporal variability of meiofauna community structure in abandoned salina of Velike soline and adjacent area (Mediterranean, Adriatic Sea). *Fresenius Environ Bull* **20** (2011) 645.
7. Nerlović V, Doğan A, Hrs-Brenko M. Response to oxygen deficiency (depletion): Bivalve assemblages as an indicator of ecosystem instability in the northern Adriatic Sea. *Biologia (Bratislava)* **66** (2011) 1114.



ORGANISATION OF THE CENTRE

Head: Karolj Skala

The Centre for Informatics and Computing Science (CIR) consists of the following units:

- ⇒ Optoelectronics and Visualisation Laboratory,
- ⇒ Department for R&D of ICST systems,
- ⇒ Department for Information systems,
- ⇒ IT Services Department



OVERVIEW OF THE DIVISION

The mission of the Centre is scientific research and the development and maintenance of infrastructure, technology and logistics for contemporary multidisciplinary (RBI) and multi-institutional (global) scientific research. Using modern computer technologies and informatics this has resulted in the development of eScience technologies based on Science Information Communication Technology—ICST. The Centre's main long-term research programme based on eScience, parallel process modelling, experimental high performance computers and computer interconnected equipment demonstrates our ex-

perience in all aspects of computer science and electronics, including scientific research, rapid prototyping design and development.

RBI/CIR is involved in several Grid and Cloud related projects in the areas of meta-computing technology, distributed computing testbed, high-speed computing, high throughput computing, virtual laboratory (teleimmersion), e-Science centre etc.

CIR expertise and experience will be of great benefit for the eCloudMan project initiatives in distributed and parallel computing and in application and service deployment, achieved through collaborations on the numerous projects listed above. The Centre's specific expertise in HPC, cluster, and GPU computing management will be of great use in the trials and validation package. CIR scientists are working on the CloudMan and Galaxy on the Cloud projects with the goal of establishing complete and easily accessible (bioinformatics) analysis environments on the cloud. CIR also acts as a work package leader on several EU6/7 projects.

TOP ACHIEVEMENTS

4D Thermography Imaging System

The camera is a multidimensional and multi-spectral camera that creates a 3D model with a temperature surface area (texture) of the observed object. This integrated broadband imaging system will be applied to medical diagnostic purposes. Successful Project - PoC BICRO (Fig. 1).

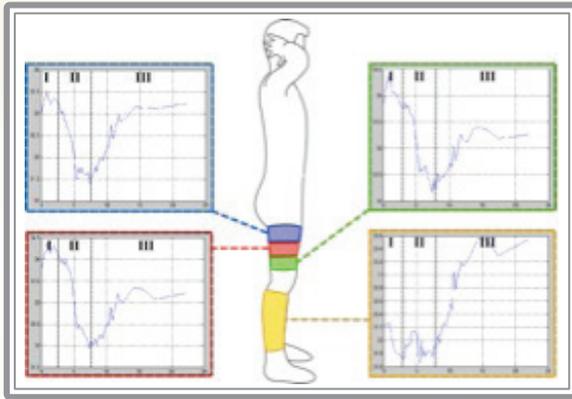


Fig.1. 4D thermal dissipation functions

NEW EQUIPMENT

New equipment developed through CIR R&D activity (BICRO project), 4D thermography imaging system (Fig 2).

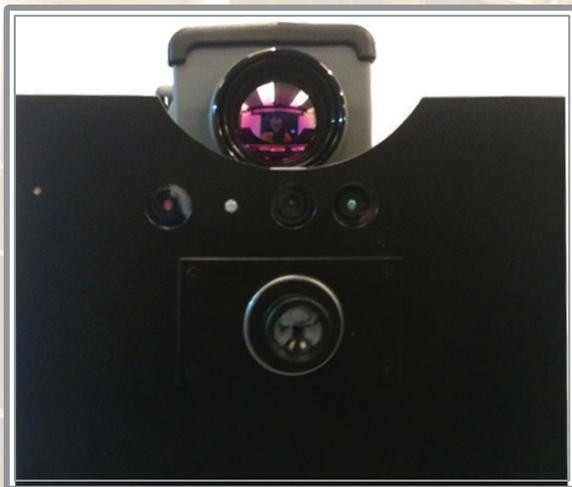


Fig. 2. 4D imaging system

EDUCATION

Members of the CIR provided bachelors and masters level courses at the University of Zagreb, Faculty of Graphic Arts, and PhD level courses at the University of Zagreb, Faculty of Electrical Engineering and Computing, University of Zagreb Faculty of Graphic Arts and University Josip Juraj Strossmayer, Osijek. In addition, CIR provided courses in Business Management at the Baltazar Adam Krčelić high school in Zaprešić.

Research program supported by the Ministry of Science, Education and Sport

1. Distributed Computing and Visualisation, Karolj Skala

Research project supported by the Ministry of Science, Education and Sport

1. Scientific project: Scientific Visualisation Methods (2007-2011), Karolj Skala

AWARDS



Fig3. Certificate

1. Enis Afgan: Ruđer Bošković RBI Director's Annual Award for a publication in a high impact factor journal. The article titled "Harnessing cloud computing with Galaxy Cloud"

was published in Nature Biotechnology (IP: 31.1) describes the integration of Galaxy and CloudMan projects.

2. Confirmation of successful completion of project for testing an innovative concept of 4D thermography (Fig 3)

ORGANIZATION OF CONFERENCE

1. 34th International Convention MIPRO, CONFERENCE on GRID AND VISUALISATION

SELECTED PUBLICATIONS

1. Skala K, Lipić T, Sović I, Gjenero L, Grubišić I. 4D Thermal Imaging System for Medical Applications. *Period Biol* **113** (2011) 407.
2. Sović I, Lipić T, Gjenero L, Grubišić I, Skala K. Artificial sets for heat source parameter estimation from 3D thermograms. *Period Biol* **113** (2011) 417.
3. Skala Kavanah H, Dubravić A, Grazio S, Lipić T, Sović I. Computer supported thermography monitoring of hand strength evaluation by electronic dynamometer. *Period Biol* **113** (2011) 433.

PUBLICATIONS PRESENTED ON CONFERENCES

1. Bojčić I, Lipić, Tomislav; Kušek, Mario; Ježić, Gordan. Extending the JADE Agent Behaviour Model with JBehaviourTrees Framework.

Proceeding of the KES-AMSTA'11 Proceedings of the 5th KES international conference on Agent and multi-agent systems: technologies and applications. Lecture Notes in Computer Science 6682 (2011)159.

2. Grubišić I, Gjenero L, Lipić T, Sović I, Skala K. Active 3D scanning based 3D thermography system and medical applications, MIPRO 2011 Rijeka, Croatia: *Proceedings of the 34th International Convention on Information and Communication Technology, Electronics and Microelectronics 1* (2011): MEET&GVS, 300.
3. Sović I, Lipić T, Gjenero L, Grubišić I, Skala K. Heat source parameter estimation from scanned 3D thermal models. MIPRO 2011: MIPRO 2011 Rijeka, Croatia: *Proceedings of the 34th International Convention on Information and Communication Technology, Electronics and Microelectronics 1* (2011): MEET&GVS, 283.
4. Borojević N, Kolarić D, Grazio S, Grubišić F, Antonini S, Nola AI, Herceg Ž. Thermography of Rheumatoid Arthritis and Osteoarthritis. PROCEEDINGS ELMAR-2011, Božek J, Grgić M (eds). Zadar : Croatian Society Electronics in Marine-ELMAR (2011) 293.

CHAPTER IN BOOKS

1. Lučić B, Sović I, Plavšić D, Trinajstić N. Hairy Matrices: Definitions, Properties and Applications. Distance in Molecular Graphs – Applications. Gutman I, Furtula B (eds). Kragujevac: University of Kragujevac and Faculty of Science Kragujevac (2011) pp 101.



ORGANIZATION OF THE CENTRE

Head: Vilko Smrečki (Dejan Plavšić until September 30, 2011)

The NMR Centre consists of the following laboratories:

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



OVERVIEW OF THE CENTRE

The mission of the Centre is to conduct scientific research in the field of NMR spectroscopy and provide services to scientists and researchers at the Ruđer Bošković Institute and the Universities of Zagreb, Rijeka, Split and Osijek. The Centre also provides educational and professional support to researchers at government institutions and in the pharmaceutical industry.

The Glass Group conducts research on the charge carriers transport phenomenon in mixed ion-electron conducting glasses. The electrical conductivity of super ionic glasses like LiI-AgI-B₂O₃ doped with transition metal ions has been the subject of extensive investigation due to their potential applications in solid state batteries.

TOP ACHIEVEMENTS

Development of NMR techniques

A constant-time TOCSY difference experiment for the determination of $^3J(^1\text{H}_3, -^{31}\text{P})$ coupling constants in non-isotope-labelled DNA oligonucleotides was developed. The new method delivers up to three times the sensitivity compared with previously reported methods (Reith et al., 2011).

Modulation of hepatoprotection by means of an antisense peptide

It was shown that an antisense peptide binds to its complementary peptide (α -MSH) and abolishes its protective effects. Tryptophan spectrofluorometric titration represents a simple and efficient method to evaluate sense-antisense peptide interaction *in vitro* (Houra et al., 2011).

The role of vanadium valence state and coordination on electrical conduction in lithium iodide borate glasses

Conductivity measurements of $\text{LiI-AgI-B}_2\text{O}_3$ have indicated that there is a mixed, both ionic and electronic, conduction. The ionic conduction seems to be dominant over polaron hopping only in glasses containing V_2O_5 at greater than 0.8 mol % of V_2O_5 . The frequency and temperature dependence of the electrical modules as well as the dielectric loss parameters have exhibited a relaxation character attributed to the vanadyl complexes (Srilatha et al., 2011).

EDUCATION

Members of the NMR centre are involved in providing bachelor level courses at the University of Rijeka and School of Dentistry, University of Zagreb, as well as providing PhD level courses at the Faculty of Science and School of Medicine University of Zagreb, University of Rijeka and Ruđer Bošković Institute. The NMR centre is also involved in the joint doctoral programs provided by the Ruđer Bošković Institute and the University of Osijek, the University of Dubrovnik, the Faculty of Medicine, University of Rijeka and at the Faculty of Science University of Split. NMR centre members also supervised 5 PhD theses defended at the Faculty of Science, Faculty of Electrical Engineering and Computing, and Faculty of Pharmacy and Biochemistry, University of Zagreb.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Influence of structure on electrical properties of (bioactive) glasses/ceramics, Andrea

Moguš-Milanković

2. NMR spectroscopy and modelling of bioactive molecules, Dejan Plavšić
3. Modelling of bioactive molecules and testing of their properties and activity, Nikola Štambuk

Research, developmental and international projects

1. Investigation of relationships between structure and biological activity of polyphenols, bilateral Croatian-Serbian project, Bono Lučić
2. Investigation of electrical mobility and dielectric relaxation of bioactive glass, bilateral Croatian-Slovenian project, Andrea Moguš-Milanković
3. NMR Study of the Interactions of Angiotensin II Receptor Antagonists, bilateral Croatian-Slovenian project, Marijana Vinković
4. Crystallization Impact on Magnetic Properties of Iron Phosphate Polaron Glasses, Croatian National Science Foundation project, Luka Pavić

SELECTED INVITED LECTURES

1. Šantić A. Charge carrier transport in materials with disordered structures. «The Twentieth Croatian-Slovenian Crystallographic Meeting – CSCM20», Baška, Island of Krk, Croatia, June 15-19, 2011.
2. Vikić-Topić D. Distribution of Lead in Ecosystem and Human Body. «Ecological Problems of Transportation Development». Croatian Academy of Sciences and Arts, Zagreb, February 24, 2011.

SELECTED ORGANIZED CONFERENCES

The 26th International Course & Conference MATH/CHEM/COMP 2011, Dubrovnik, Croatia, June 13-18, 2011.

SELECTED PUBLICATIONS

1. Randić M, Zupan J, Balaban AT, Vikić-Topić D, Plavšić D. Graphical Representation of Proteins. *Chem Rev* **111** (2011) 790.
2. Šagud I, Faraguna F, Marinić Ž, Šindler-Kulyk M. Photochemical approach to naphthoxazoles and fused hetero-benzoxazoles from 5-(phenyl/heteroarylethenyl)oxazoles. *J Org Chem* **76** (2011) 2904.
3. Reith LM, Schlagnitweit J, Smrečki V, Knoer G, Mueller N, Schoefberger W. Determination of $^3J(^1H_3-^{31}P)$ couplings in a DNA oligomer with enhanced sensitivity employing a constant-time TOCSY difference experiment. *Magn Reson Chem* **49** (2011) 125.
4. Brnčić M, Bosiljkov T, Ukrainczyk M, Tripalo B, Rimac Brnčić S, Karlović S, Karlović D, Ježek D, Vikić-Topić D. Influence of whey protein addition and feed moisture content on chosen physico-chemical properties of directly expanded corn extrudates. *Food Bioprocess Tech* **4** (2011) 1296.
5. Šantić A, Skoko Ž, Gajović A, Reis ST, Day DE, Moguš-Milanković A. Physical properties of lead iron phosphate glasses containing Cr_2O_3 . *J Non-Cryst Solids* **357** (2011) 3578.
6. Houra K, Turčić P, Gabričević M, Weitner

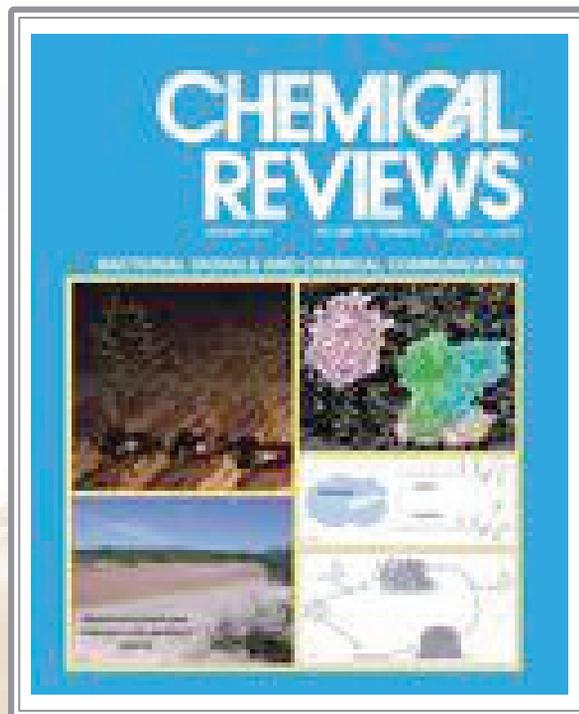


Fig. 1.

T, Konjevoda P, Štambuk N. Interaction of α -melanocortin and its pentapeptide anti-sense LVKAT: Effects on hepatoprotection in male CBA mice. *Molecules* **16** (2011) 7331.



Head of Library: Bojan Macan

OVERVIEW OF LIBRARY ACTIVITIES

The mission of every research library is to support research and learning through the provision of access to the world's knowledge base. In the print environment, this mission was pursued by ensuring that library users had access to all of the print resources purchased by the library.

With the development of the Internet and Web, new possibilities have emerged for libraries and scientific communication in general. The RBI Library recognized the potential of Open Access and continued to promote it and ease access to OA literature, as well as access to subscribed peer-reviewed journal literature for the whole Croatian academic community. The Library also continued to work on improving its new website and adding new content. During 2011 the Library wrote 200 news items on its Blog (<http://knjiznica.irb.hr/blog>) covering various subjects - from scientific to popular and cultural ones. The Library disseminated news using the Library's Facebook profile (<http://www.facebook.com/irb.knjiznica>), as well as Twitter profile (<http://twitter.com/irblibrary>), where the Library has a few hundred regular followers.

In order to connect more closely and directly with online users, the Library launched a new service on their website called "Live chat" where users can contact librarians via chat software implemented on the Library's website. The Library also installed and tested



a BigBlueButton teleconference system and offered it to the public free of charge (<http://conf.irb.hr>).

Work on the institutional repository included rearrangement of the metadata schema. Document deposition was tested and best practices were carefully examined to avoid problems during repository launching.

In 2011 a new Library Board was convened and, in coordination with the Board, new Library legislation was drafted and sent to the Institute's management for further deliberation and approval.

During 2011 the Library worked on improving and maintaining the open source integrated library system Koha. The new release, including adjustments, was implemented. At the same time preparations for data import of the journal collection from

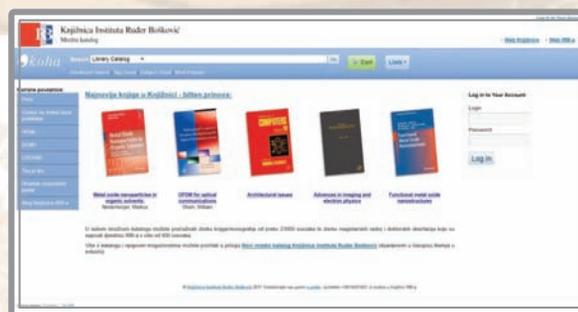


Figure 1: Library's Online Public Access Catalog (Koha)

the current SAND database were made. In order to better inform users about new acquisitions in the Library, an application was created which displays the covers of newly acquired books on the Library homepage, as well as on the homepage of the Library's Online Public Access Catalogue, (<http://katalog.irb.hr>).



Figure 2: A Pair of Compasses (ŠESTAR), Library's database of scientific instruments

To ensure documentation of RBI's capital equipment, development continued on the repository of research instruments ŠESTAR (A Pair of Compasses). Several improvements were made including availability of an English language version and a reservation module. Using the XML metadata schema, specifications and information on instruments will in future be available through the RBI web site.

COLLECTION DEVELOPEMENT

Access to the collection of e-journals (ScienceDirect) and e-databases via the Ministry of science, education and sport subscription for the whole Croatian academic community was partially unavailable during this year, due to non-renewal of subscriptions. In addition to these national subscriptions and open access journals, the Library subscribed to 233 e-journals, 48 printed journals (subscription to selected titles from different publishers, as well as to e-journal packages from

IOP and Emerald) as well as the Faculty of 1000 database. Quick access to all available e-journals was provided via the Pero search engine for e-journals (<http://knjiznica.irb.hr/pero/>) as well as through EZB Elektronische Zeitschriftenbibliothek (<http://lib.irb.hr/web/hr/casopisi/item/202-ezb.html>).

All literature acquisitions at the Institute were processed by the Library. In 2011 the Library acquired 301 new books, and therefore the collection of all books now counts 23.249 volumes in total. The collection of RBI theses includes 451 volumes of Ph. D. theses and 423 volumes of M.Sc. theses.

The RBI Library was actively involved in the celebration of the 300th anniversary of the birth of Josip Ruđer Bošković's. To promote J. R. Bošković's life and work, a special collection was exhibited in the Library reading room in the 5th wing. So far the Library has collected around 30 Croatian and foreign titles including rare print editions of J. R. Bošković's books. New books published or edited by RBI scientists were donated to the Library's special collection by the authors.

LIBRARY SERVICES

With new technological developments and innovations, come new challenges and new expectations. The RBI Library continued to

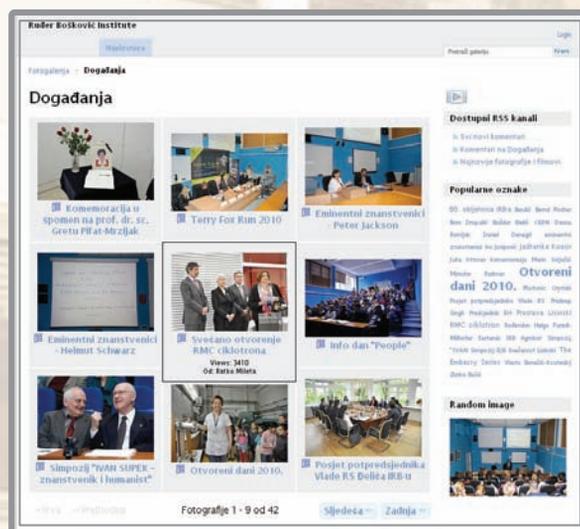


Figure 3: Publicly available RBI Photo gallery

maintain their services, and to monitor how researchers have been making use of those services. While usage of library resources and services was high, financial support was lacking this year. Plans for improvements to existing information services as well as introduction of new services remained mostly unfilled:

- Search engine of e-journals – Pero (<http://knjiznica.irb.hr/pero/>) – major improvements needed, monitoring tool, currency tool;
- EZB Elektronische Zeitschriftenbibliothek (<http://lib.irb.hr/web/hr/casopisi/item/202-ezb.html>) – up to date;
- Croatian Scientific Bibliography – CROSBI (<http://bib.irb.hr>) – major improvements needed, interoperability tools, monitoring tools, authority tools;
- Who is Who in Croatian Science (<http://tko-jetko.irb.hr>) – complete revision needed;
- Centre for Online Databases (<http://www.online-baze.hr>) – better communication at different levels and more transparency needed;
- CMS for web sites of Croatian academic and research libraries (<http://knjiznice.szi.hr>) – complete revision and portability needed;
- IRB reservations (<https://rezervacije.irb.hr>) – up-to date
- Library's photo gallery (<http://lib.irb.hr/fotoarhiv/>) and publicly available RBI Photo gallery (<https://lib.irb.hr/fotogalerija/>) – merging of those two galleries, migration to new platform and more detailed metadata description needed.

Through cooperation with the University of Zadar, administration support was provided by LIS students working on CROSBI and Who's Who in Science in Croatia. Student support was of great help in the given circumstances.

In 2011 the Library worked on revising the functionalities and processes of an in-house developed application for interlibrary loan service – SEND (<http://send.irb.hr>). Documentation and plans for the new application were

elaborated and in the forthcoming period a new and improved application should be programmed and published. This new application should be made available to other Croatian libraries.

Bibliometric analysis for RBI

Citation and bibliographic databases Web of Science, Scopus, Google Scholar, SPIRES and Current Contents were used for bibliometric analysis and in 2011 a total of 94 citation certificates were issued to RBI scientists for advancement purposes. The Library would like to offer this service in future to the whole academic community for a fee.

Interlibrary Loan

The RBI library has a well established interlibrary loan and lending service with libraries from Croatia and abroad. Interlibrary loan services from other Croatian libraries as well as from EURASLIC/IAMSLIC libraries are mainly free of charge, while copy and loan requests from libraries abroad are charged (e.g. SUBITO catalogue of German libraries). In 2011 the RBI library received a slightly increased number of interlibrary loan requests for document delivery by RBI staff due to the difficulties in access to 2011 content of ScienceDirect journals. In 2011 the Library received 1033 requests for document delivery by RBI staff in total and 812 (79%) of those requests were positively resolved. In 2011 most items were obtained through the IAMSLIC catalogue (458, 44%) followed by SUBITO (165, 16%). The majority of requested documents were acquired free of charge (77% of positively resolved requests).

The RBI library also received 623 requests for document delivery from other Croatian libraries, and positively resolved 82% of those requests.

In 2011 the Library continued with its user education program and its short educational library seminars called KEKS (Kratki edukacijski knjižnični seminari, in Croatian). KEKS seminars consist of short lectures (45 minutes) and an hour and a half or two hour workshops. KEKS seminars are held periodically in small groups with a maximum of 10 participants in order to enable an individual approach to each participant. Seminars take place in one of the Library's reading rooms, with the use of laptops. Usually seminars are held in Zagreb, but in 2011 the KEKS seminars were also offered to RBI scientists in Rovinj. Twenty one seminars were held in 2011 with 98 participants in total. Due to the great interest for KEKS seminars among Croatian librarians and research staff from other institutions, the Library is planning to offer KEKS seminars in the future as a service for non RBI staff for a symbolic fee. Before doing so, the new Library legislative framework must be adopted.

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

International cooperation

International cooperation with EURASLIC (European Association of Aquatic Sciences Libraries and Information Centers) and its parent organization IAMSLIC (European Association of Aquatic Sciences Libraries and Information Centres) continues. The Library had an active role in EURASLIC activities, as well as in its subgroups the ECET (European Countries in Economic Transition) group and the MedSig group (The Mediterranean Special Interest Group), as well as the IAMSLIC Strategic Planning Group.

The Library participated in training courses held at the UNESCO/IOC Project Office for IODE in Oostende, Belgium. In 2011 two grants for training courses were received:

- Joint ODINECET/ODINBlackSea Work-

shop, September 12th - 14th, 2011, Sevastopol, Ukraine

- Training Course on Outreach and Communication Tools, November 7th – 11th, 2011, Oostende, Belgium

Thanks to these grants two persons from the library staff participated in the 14th Biennial Conference, Lyon, France, May 17-20, 2011. Previous to this conference, two members of the library staff were members of the EURASLIC board. Following the Conference one RBI library staffer was appointed to the new board as Executive secretary, (website and newsletter editor).

Organization of events

During 2011 the Library organized two book exchanges under the title "Take it or leave it". RBI employees brought their used books in and exchanged them for other books. During this event about 500 books were exchanged, and any remaining books were offered as donations to other libraries.

The Library also continued to organize the RBI Library Colloquia. Colloquia topics covered a wide range of topics chosen to be of interest not only to librarians, but also to RBI staff and the general public. During this year seven lectures were organized.

UZMI ILI OSTAVI

RAZMJENA KNJIGA U KNJIŽNICI IRB-a
– za djelatnike Instituta –

Kod kuće imate pune police pročitanih knjiga koje sakupljaju prašinu? Tražite mudro
štivo za čitanje tijekom hladne zime? Posjetite našu razmjenu knjiga!



GDJE: Knjižnica IRB-a, 1. krilo

KADA: 29.11. - 2.12. (utorak - petak)

Moguće sve kombinacije uzimanja/ostavljanja
(samo uzmi, samo ostavi ili oboje ☺)

Detalji na Blogu Knjižnice:
<http://lib.irb.hr/web/hr/blog.htm>

Figure 4: "Take it or leave it" - exchange of books in RBI Library

PROJECTS

In 2011 the Library became a partner in its first FP7 project called 2nd Generation Open Access Infrastructure for Research in Europe - OpenAIREplus (under the Infrastructure Call 9). This project will build a 2nd-Generation Open Access Infrastructure by significantly expanding the outcomes of the OpenAIRE project and, in addition, generically harvesting and indexing the metadata of scientific datasets in selected diverse OA thematic data repositories. This project officially started on November 1st 2011 and will last for 30 months.

In 2011 individual Library staff were active in applying for a FP7 project called Support for Establishment of National/Regional Social Sciences Data Archives (SERSCIDA) which has been approved and is currently in the process of negotiations. SERSCIDA is engaged with the development of digital archives of original research data in the field of social sciences. Library staff were also active as collaborators on the IPA project Development of Innovation System at Ruđer Bošković Institute and University of Rijeka.



Figure 5: OpenAIREplus - Library's first FP7 project

SELECTED PUBLICATIONS

1. Macan B, Konjević S. A survey of interlibrary loans at Ruđer Bošković Institute Library, Croatia, 2003-2008. *Interlend Doc Supply* **39** (2011) 45.
2. Macan B. Bibliometric analysis of the journal *Kemija u industriji* for the period 2000 - 2009. *Kem Ind* **60** (2011), 81-88. (in Croatian)
3. Pažur I: E-book reader devices and libraries. *Kem Ind* **60** (2011) 157. (in Croatian)
4. Konjević S, Mayer M. Caught in the "Fishing Net" of Information - 14th biennial EURASLIC conference. 28th OMER Conference. *Kem Ind* **60** (2011) 461. (in Croatian)
5. Mayer M. 2011 - International year of chemistry. *Kem Ind* **60** (2011) 229. (in Croatian)

SELECTED LECTURE

1. Konjević S. Interlibrary Loan at Ruđer Bošković Institute Library, Croatia, 2009-2010. Caught in the "fishing net" of information: 14th Biennial Meeting of the European Association of Aquatic Science Libraries and Information Centres (EURASLIC) and 28ème conférence annuelle OMER, Lyon, France, May 17-20, 2011.
2. Mayer M. RBI Library New Web. Caught in the "fishing net" of information: 14th Biennial Meeting of the European Association of Aquatic Science Libraries and Information Centres (EURASLIC) and 28ème conférence annuelle OMER, Lyon, France, May 17-20, 2011.

Notes





